nature chemistry

SUPPLEMENTARY INFORMATION

DOI: 10.1038/NCHEM.749

Highly stable TTF radical dimers in [3]catenanes

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1. General Methods

All reagents were purchased from commercial suppliers (Aldrich or Fisher) and used without further purification. Cyclobis(paraquat-4,4′-biphenylene) tetrakis(hexafluorophosphate)[S1] (**1**·4PF_6), 4,4′(5′)-bis[2-(2-{2-(propargyl)ethoxy}ethoxy)ethoxy]tetrathiafulvalene[S2] (**7**), the TTF/DNP macrocycle[S3] **4**, and 1,1′-[4,4′-biphenylenebis-(methylene)]bis(4,4′-bipyridinium) bis(hexafluorophosphate)[S4] (**5**·2PF_6) were prepared according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F_{254} (E. Merck). Column chromatography was performed on silica gel 60F (Merck 9385, 0.040-0.063 nm). Nuclear magnetic resonance (NMR) spectra were recorded at 25 ˚C (unless otherwise noted) on Bruker Avance 500 and 600 spectrometers, with working frequencies of 500 and 600 MHz for ^{1}H, and 125 and 150 MHz for ^{13}C nuclei, respectively. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents[S5]. All ^{13}C spectra were recorded with the simultaneous decoupling of proton nuclei. UV-Vis-NIR absorbance spectra

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were recorded using a Perkin Elmer LAMBDA 1050 double beam, double monochromator, ratio-recording spectrometer. EPR Measurements at X-band (9.5 GHz) were made using a Bruker Elexsys E580. The EPR spectrometer was equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). Steady-state CW EPR spectra were measured using 0.2–2 mW microwave power and 0.01–0.05 mT field modulation at 100 KHz, with a time constant of 5.12 ms and a conversion time of 40.96 ms. Electrospray Ionisation (ESI) mass spectra were obtained on a Agilent 6210 LC-TOF high resolution mass spectrometer. Nanoelectrospray HRMS spectra were collected on a ThermoElectron LTQ-FT-MS. Cyclic voltammetry experiments were performed on a Princeton Applied Research 263 A Multipurpose instrument interfaced to a PC, using a glassy carbon working electrode (0.018 cm^2, Cypress system). The electrode surface was polished routinely with 0.05 μm^2 alumina/water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was a AgCl coated Ag wire. The concentrations of the samples were 1 mM in 100 mM electrolyte solution (NBu_4PF_6 in MeCN).

2. Computational Methods

Calculations were performed on all systems using density functional theory (DFT) with the M06-L and M06-2X functionals, as implemented[S6] in Jaguar 7.6r110. Starting with a structure from the crystallographic data, we optimised the geometry using the 6-31G** basis set with the M06-L functional in the gas phase. Single-point energies were calculated using the M06-2X functional and the 6-31G** basis set. Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for acetonitrile (ε = 37.5, R_0= 2.18 Å) using the PBF module in Jaguar.

3. Synthesis

2·4PF$_6$: The macrocycle **4** (300 mg, 0.40 mmol) and **5**·4PF_6 (158 mg, 0.20 mmol) were dissolved in DMF in the presence of 1,1′-bis(bromomethyl)-4,4′-biphenyl (**6**) (72 mg, 0.21 mmol) and stirred for 14 days at room temperature under a N_2 atmosphere. The solvent was removed *in vacuo* and the green solid was subjected to chromatography (SiO_2, MeOH : 2M NH_4Cl : $MeNO_2$ (7:2:1) eluent). The fractions containing the [2]- and [3]catenanes were each

combined, the solvent removed *in vacuo*, and treated with cold H_2O and an excess of NH_4PF_6 to precipitate the [2]catenane (20 mg, 5%) and **2**·4PF_6 (167 mg, 33%), respectively. **2**·4PF_6: ^{1}H NMR (600 MHz, CD_3COCD_3, 300 K): δ 9.02 (d, $^3J_{HH}$ = 6.5 Hz, 8H, α-bipy$^+$-H), 7.76 (d, $^2J_{HH}$ = 8.5 Hz, 8H, phenylene-H), 7.70 (d, $^2J_{HH}$ = 8.5 Hz, 8H, phenylene-H), 7.43 (d, $^3J_{HH}$ = 6.5 Hz, 8H, β-bipy$^+$-H), 7.30–7.08 (br m, 8H, DNP-H (3/7, 2/6)), 6.70 (d, $^3J_{HH}$ = 7 Hz, 4H, DNP-H (4/8)), 5.99 (s, 8H, macrocyclic CH_2), 5.95 (s, 4H, SC*H*), 4.08 (br s, 8H, SCCH_2), 3.98–3.92 (br m, 24H), 3.90 (m, 16H), 3.81 (s, 16H), 3.71 (m, 8H); ^{13}C NMR (150 MHz, CD_3COCD_3, 300 K): δ 154.8, 145.1, 144.0, 141.9, 133.8, 133.7, 131.2, 128.8, 126.7, 126.6, 124.7, 119.3, 114.7, 110.4, 106.5, 72.1, 71.9, 71.6, 71.1, 70.6, 68.6, 65.7; HRMS (ESI) Calcd for $C_{116}H_{128}F_{24}N_4O_{20}P_4S_8$: *m/z* = 2587.5812 ([*M* − PF_6]$^+$), 1221.3085 ([*M* − 2PF_6]$^{2+}$), 765.8843 ([*M* − 3PF_6]$^{3+}$), 538.1722 ([*M* − 4PF_6]$^{4+}$); Found: *m/z* = 1221.3092 ([*M* − 2PF_6]$^{2+}$), 765.8849 ([*M* − 3PF_6]$^{3+}$); mp 165–169 °C with decomposition.

3·4PF_6: $Cu(OAc)_2·H_2O$ (40.0 mg, 0.200 mmol) was added to a green solution of **7** (121 mg, 0.200 mmol) and **1**·4PF_6 (50.0 mg, 0.040 mmol) dissolved in MeCN (30 mL) and the solution was stirred for 72 h under ambient conditions. The solvent was removed *in vacuo* and the green residue was subjected to chromatography (SiO_2, MeOH : 2M NH_4Cl : $MeNO_2$ (7:2:1) eluent). The green band was collected, concentrated *in vacuo*, and treated with cold H_2O and an excess of NH_4PF_6 to precipitate a green solid (49.2 mg, 50%). **3**·4PF_6: ^{1}H NMR (600 MHz, CD_3CN, 293 K): δ 9.21–9.04 (m, 8H, α-bipy$^+$-H), 7.95–7.79 (m, 8H, β-bipy$^+$-H), 7.66–7.60 (m, 16H, phenylene-H), 5.95 (s, 4H, SC*H*), 5.79–5.70 (m, 8H, macrocyclic CH_2), 3.96–3.91 (m, 8H, SCCH_2), 3.89 (s, 8H, C≡CCH_2O), 3.85–3.83 (m, 8H), 3.82–3.79 (m, 8H), 3.77–3.75 (m, 8H), 3.73–3.70 (m, 8H), 3.69–3.66 (m, 8H), 3.61–3.58 (m, 8H), 3.36–3.33 (m, 8H); ^{13}C NMR (125 MHz, CD_3CN, 293 K): δ 145.8, 145.3, 142.0, 133.7, 133.6, 131.0, 129.0, 126.7, 125.7, 119.7, 110.6, 77.3, 76.8, 72.2, 71.8, 71.4, 71.2, 71.1, 71.0, 71.0, 70.9, 70.5, 70.1, 69.8, 68.7, 68.3, 65.5, 59.3, 59.2; HRMS (ESI) Calcd for $C_{100}H_{108}F_{24}N_4O_{16}P_4S_8$: 2311.4402 ([*M* – PF_6]$^+$), 1083.2405 ([*M* – 2PF_6]$^{2+}$), 673.8389 ([*M* – 3PF_6]$^{3+}$), 469.1382 ([*M* – 4PF_6]$^{4+}$), Found: 2311.4394 ([*M* – PF_6]$^+$), 1083.2416 ([*M* – 2PF_6]$^{2+}$), 673.8392 ([*M* – 3PF_6]$^{3+}$), 469.1385 ([*M* – 4PF_6]$^{4+}$); mp 152–156 °C with decomposition.

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4. Crystallisation

All crystallographic data has been deposited with the Cambridge Crystallographic Data Centre as supplementary publications, and are available free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Single crystals of $(TTF_2 \subset \mathbf{1})\cdot 4TTF \cdot 4PF_6$ were grown by slow evaporation from MeCN. Intensity data were collected on a Bruker P4 four circle serial diffractometer (MoKα radiation) cooled by an Oxford Cryosystems Cryostream.

Crystal data for $(TTF_2 \subset \mathbf{1})\cdot 4TTF \cdot 4PF_6$. $C_{84}H_{64}N_4S_{24}\cdot(PF_6)_4$. Red plate (0.78 × 0.64 × 0.18 mm). *Cc*, a = 28.643(5), b = 14.210(5), c = 24.502(5) Å, β = 99.380(5)°, V = 9839(4) Å^3, Z = 4, T = 160(2) K, ρ_{calc} = 1.673 gcm^{-3}, μ = 0.680 mm^{-1}, $F(000)$ = 5024. A total of 8807 reflections were collected, of which 8807 were unique (R_{int} = 0.0000). Final $R_1(F^2 > 2\sigma F^2)$ = 0.0785. CCDC number: 778550.

Single crystals of $\mathbf{2}\cdot 4PF_6\cdot(MeCN)_{2.5}$ and $\mathbf{3}\cdot 4PF_6\cdot(MeCN)_3$ were grown by slow vapour diffusion of *i*Pr$_2$O into solutions of the [3]catenanes in MeCN. For $\mathbf{2}\cdot 4PF_6\cdot(MeCN)_{2.5}$, intensity data were collected at 173 K using CuKα radiation with a Rigaku MM007/Saturn92 system. For $\mathbf{3}\cdot 4PF_6\cdot(MeCN)_3$, intensity data were collected at 93 K using MoKα radiation with a Rigaku MM007/Saturn70 system.

Crystal data for $\mathbf{2}\cdot 4PF_6\cdot(CH_3CN)_{2.5}$. $[C_{116}H_{128}N_4O_{20}S_8\cdot(PF_6)_4]\cdot(CH_3CN)_{2.5}$. Green prism (0.30 x 0.20 x 0.20 mm). $P2_1/c$, a = 27.049(2), b = 16.3551(18), c = 29.944(3) Å, β = 92.265(3)°, V = 13236(2) Å^3, Z = 4, T = 173(2) K, ρ_{calc} = 1.424 gcm^{-3}, μ = 2.581 mm^{-1}, $F(000)$ = 5884. A total of 23,810 reflections were collected, of which 13,770 were unique, with R_{int} = 0.1005. Final $R_1(F^2 > 2\sigma F^2)$ = 0.1263. There is some slight unresolved disorder in the ether linkages in one moiety. ISOR and DFIX restraints were used to help the refinement. Some disorder, especially in calculated hydrogen atoms was still evident. The region in question is from approx. C102 to C105 and O128 to O131. CCDC number: 778551.

Crystal data for 3·4PF$_6$·(CH$_3$CN)$_3$. [$C_{100}H_{108}N_4O_{16}S_8$·$(PF_6)_4$]·$(CH_3CN)_3$. Green platelet (0.15 x 0.10 x 0.02 mm). *P*-1, a = 11.144(4), b = 14.355(5), c = 19.592(8) Å, α = 86.784(13), β = 87.155(15), γ = 75.382(13)°, V = 3025.7(19) Å^3, Z = 1, T = 93(2) K, ρ_{calc} = 1.417 gcm^{-3}, μ = 0.300 mm^{-1}, F(000) = 1334. A total of 31,322 reflections were collected, of which 6846 were unique, with R_{int} = 0.0423. Final $R_1(F^2 > 2\sigma F^2)$ = 0.1986. There was slight disorder in the solvate acetonitrile molecules which was dealt with using ISOR constraints. The TTF components were refined using DFIX instructions. CCDC number: 778552.

Single crystals of the oxidised [3]catenanes **3**·4PF$_6$·ClO$_4$ and **3**·2PF$_6$·4ClO$_4$ were prepared by titrating aliquots of a solution of Fe(ClO$_4$)$_3$ in MeCN into a solution of **3**·4PF$_6$ in MeNO$_2$. Addition of 1 equiv of Fe(ClO$_4$)$_3$ to **3**·4PF$_6$ generated the mixed-valence [3]catenane **3**$^{5+}$, while 2 equiv generated the radical cation dimer **3**$^{6+}$. Slow vapour diffusion of Et$_2$O into the solution of **3**$^{5+}$ at 0°C during 1 week resulted in the separation of red blocks of **3**·4PF$_6$·ClO$_4$, while slow vapour diffusion of Et$_2$O into the solution of **3**$^{6+}$ at -20°C during 2 months resulted in the separation of red plates of **3**·2PF$_6$·4ClO$_4$·$(CH_3NO_2)_5$·$(C_4H_{10}O)$. X-Ray diffraction data for both oxidised [3]catenanes were collected on a Bruker Kappa diffractometer, equipped with a Cu Kα sealed-tube source and an APEX II CCD detector.

Crystal data for 3·4PF$_6$·ClO$_4$. [$C_{100}H_{108}N_4O_{16}S_8$·$(PF_6)_4$·$(ClO_4)$]. Red block (0.45 x 0.26 x 0.21 mm). $C222_1$, a = 13.4168(10), b = 37.385(3), c = 27.8719(17) Å, V = 13980.2(18) Å^3, Z = 4, T = 100(2) K, ρ_{calc} = 1.215 gcm^{-3}, μ = 2.555 mm^{-1}, F(000) = 5268. A total of 12,798 reflections were collected, of which 4845 were unique, with R_{int} = 0.039. Final $R_1(F^2 > 2\sigma F^2)$ = 0.0888. The atoms of the two TTF macrocycles were subjected to SAME restraints. Global rigid bond restraints (DELU/SIMU) were also applied. The perchlorate anion was subjected to Cl—O and O—O distance restraints; it is disordered on a symmetry position which served to distort its geometry. Diffuse, disordered solvent molecules, a mixture of Et$_2$O and MeNO$_2$, could not be adequately modelled. The bypass procedure in *PLATON*[S7] was used to remove the electronic contribution from these solvents. The total potential solvent accessible void volume was 3707.9 Å^3 and the electron count / cell = 1230. As the exact solvent content is not known, the reported

DOI: 10.1038/NCHEM.749

formula reflects only the atoms used in the refinement. The structure is achiral but crystallises in the chiral space group $C222_1$. A TWIN command was included in the refinement to account for racemic twinning. The BASF parameter refined to 0.36 (5). CCDC number: 778553.

Crystal data for $3{\cdot}2PF_6{\cdot}4ClO_4{\cdot}(CH_3NO_2)_5{\cdot}(C_4H_{10}O)$. [$C_{100}H_{108}N_4O_{16}S_8{\cdot}(PF_6)_2{\cdot}(ClO_4)_4{\cdot}(CH_3NO_2)_5{\cdot}(C_4H_{10}O)$]. Red plate (0.49 x 0.32 x 0.06 mm). *P*-1, a = 14.1826(5), b = 21.4251(8), c = 22.9043(8) Å, α = 95.326(3), β = 95.544(2), γ = 92.596(2)°, V = 6887.0(4) Å^3, Z = 2, T = 100 (2) K, ρ_{calc} = 1.420 gcm^{-3}, μ = 2.990 mm^{-1}, $F(000)$ = 3056. A total of 19,091 reflections were collected, of which 4864 were unique, with R_{int} = 0.0534. Final $R_1(F^2 > 2\sigma F^2)$ = 0.0944. While several ordered $MeNO_2$ solvent molecules were found and refined, additional disordered solvent molecules, a mixture of Et_2O and $MeNO_2$, could not be adequately modelled. The bypass procedure in *PLATON*[S7] was used to remove the electronic contribution from these solvents. The total potential solvent accessible void volume was 531.7 Å^3 and the electron count / cell = 183. As the exact solvent content is not known, the reported formula reflects only the atoms used in the refinement. Global rigid bond and similarity restraints were applied to keep thermal parameters reasonable. The ordered $MeNO_2$ molecules were subjected to SAME restraints. CCDC number: 778554.

5. Titration Oxidation Studies

UV-Vis-NIR Spectra were recorded from a solution of **3**·4PF_6 (3 mL, 0.3 mM, MeCN) through a 1.0 cm path-length cuvette throughout the successive addition of a solution of $Fe(ClO_4)_3$ (2 µL aliquots, 100 mM, MeCN). Nanoelectrospray HRMS spectra were performed on solutions of $\mathbf{3}^{4+}$, $\mathbf{3}^{5+}$, $\mathbf{3}^{6+}$, and $\mathbf{3}^{8+}$ (3 µM, MeCN) prepared from the titration of $Fe(ClO_4)_3$ (50 mM, MeCN). ^{1}H NMR spectra were recorded from a solution of **3**·4PF_6 (122 µL, 2.0 µM, CD_3CN) following the successive addition of tris(4-bromophenyl)ammoniumyl hexachloroantimonate (0.4 mg aliquots). EPR Spectra were recorded on a solution of **3**·4PF_6 (854 µL, 0.5 mM, MeCN) in an unsealed quartz tube (1.4 mm I.D.) across the successive addition and mixing of a solution of $Fe(ClO_4)_3$ (4 µL aliquots, 50 mM, MeCN; the solution in the tube was removed and mixed with the parent solution and added oxidant between the recording of each spectrum).

6. 2D and VT NMR Investigations

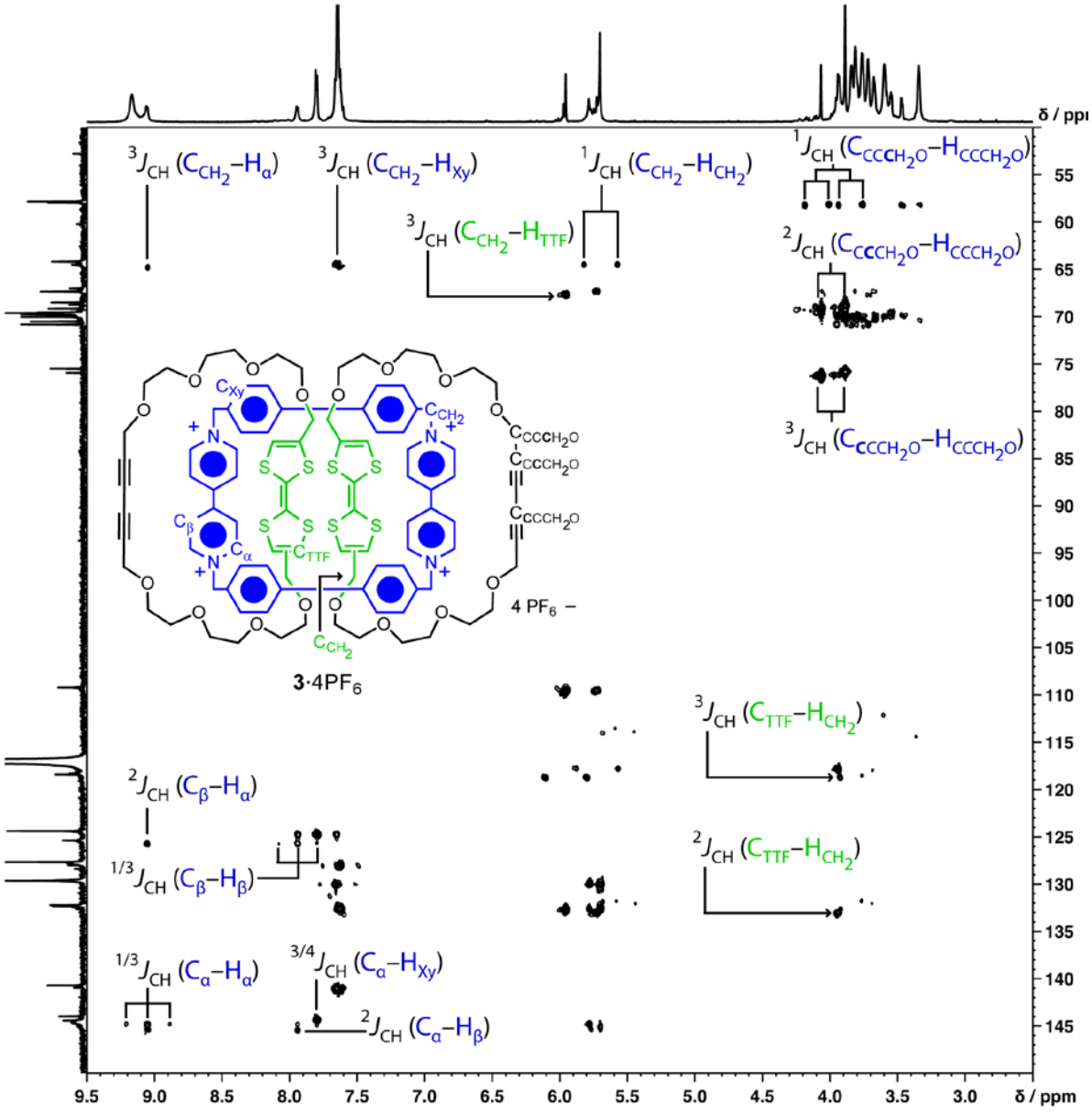

Figure S1: ^{1}H –^{13}C HMBC (with two-fold low-pass J-filter to suppress one bond correlations) NMR Spectrum of **3**·4PF_6 recorded in CD_3CN at 293K. Selected correlations (shown) were used to aid 1D ^{1}H NMR assignments.

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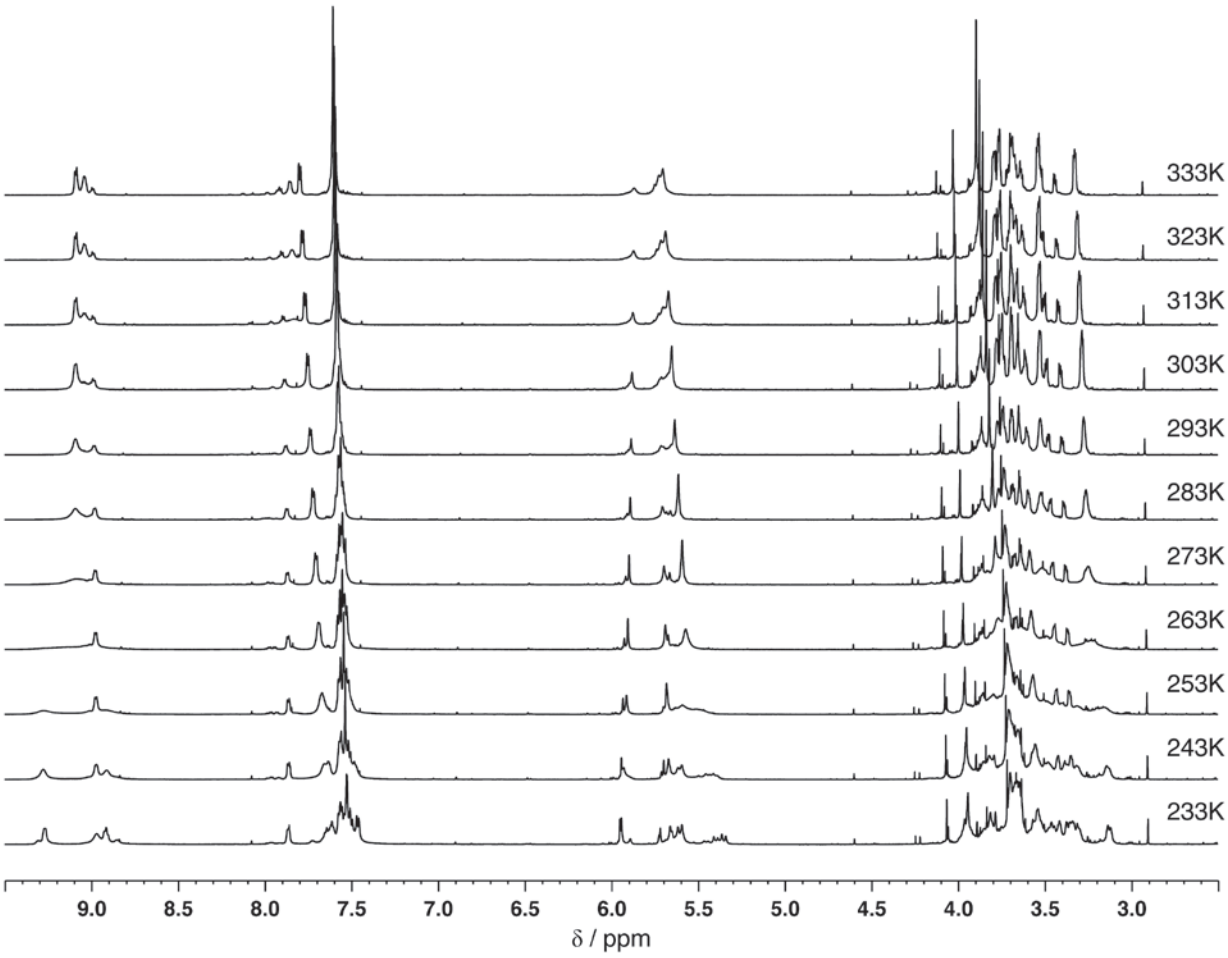

***Figure S2*:** Variable Temperature ^{1}H NMR spectra of **3**·4PF_6 (600 MHz, CD_3CN)

7. UV-Vis-NIR and ^{1}H NMR Switching Studies of 2·4PF$_6$

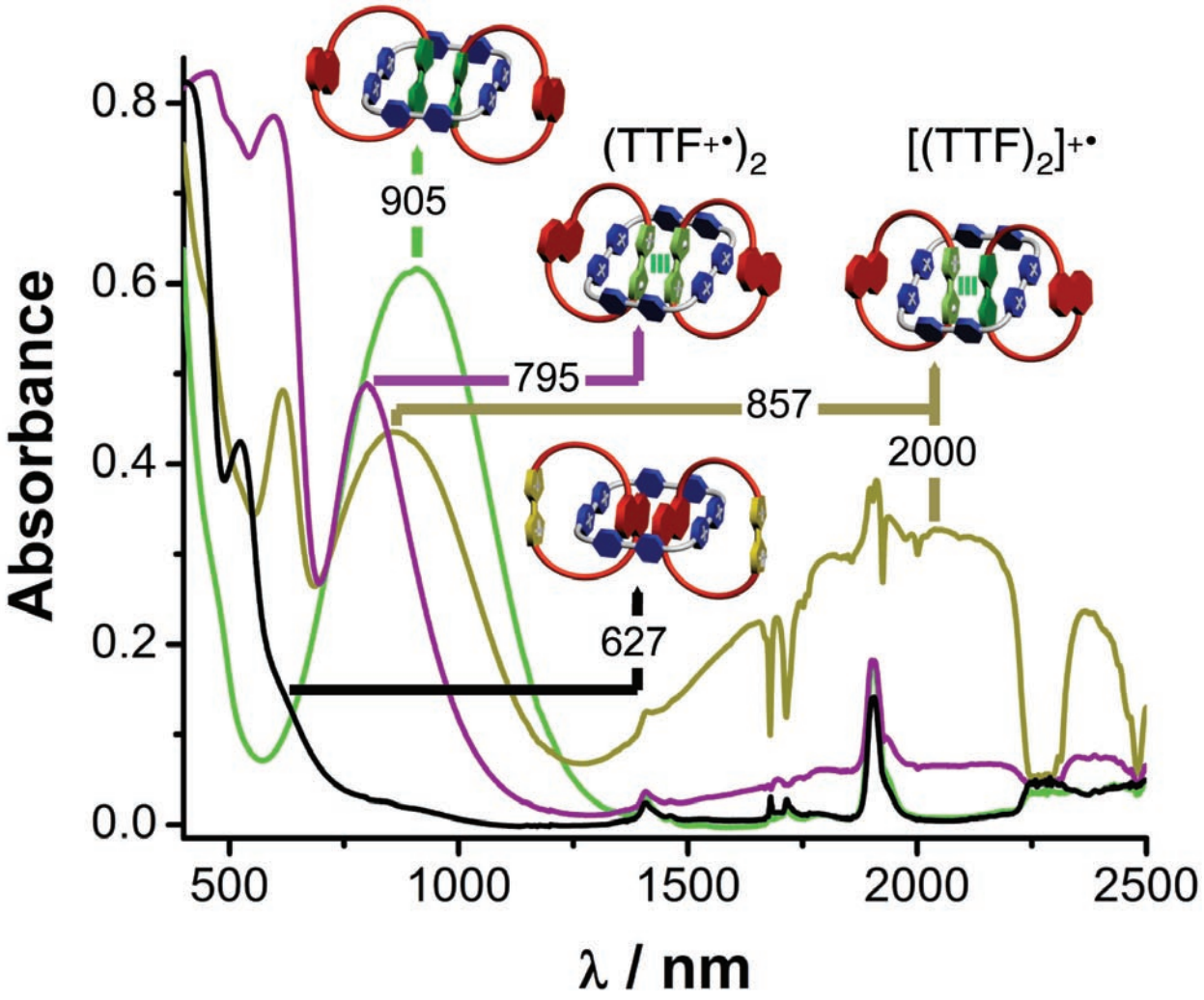

***Figure S3*:** Overlaid spectroelectrochemistry spectra of **2·4PF$_6$** after applying potentials of 0 V (green trace), 500 mV (blue trace), 800 mV (purple trace), and 1200 mV (black trace). Absorbances characteristic (highlighted graphically above) for TTF-bipyridinium charge transfer, $(TTF)_2^{\bullet+}$ mixed-valence dimers, $(TTF^{\bullet+})_2$ radical-cation dimers, and DNP-bipyridinium charge transfer are present upon each successive oxidation. All spectra were recorded from MeCN solutions of **2·4PF$_6$** (1 mM) using an optically transparent thin layer electrochemical (OTTLE) cell[S8] with an optical path of 1 mm, using a Pt grid as a working electrode, a Pt wire as counter electrode, and a Ag/AgCl reference electrode.

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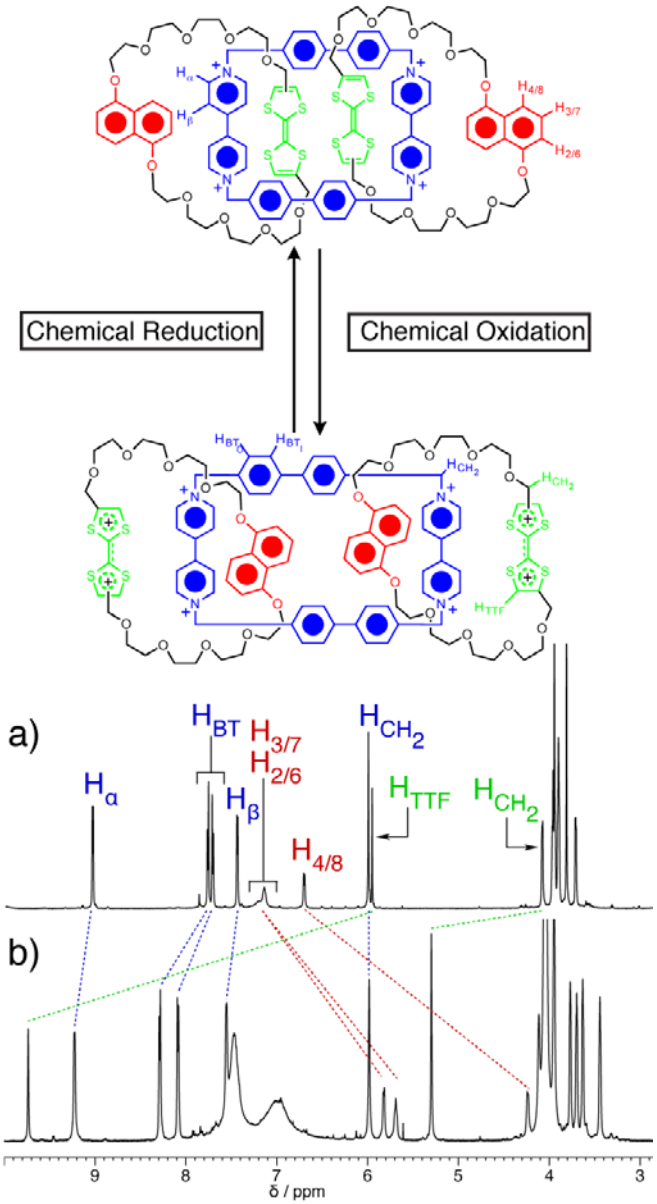

Figure S4: ^{1}H NMR spectra (600 MHz, CD_3COCD_3, 300 K) of (a) [3]catenane $\mathbf{2}^{4+}$ and (b) fully oxidized $\mathbf{2}^{8+}$ after the addition of 4.5 equiv of the chemical oxidant tris(4-bromophenyl) ammoniumyl hexachloroantimonate. The inclusion of the DNP moieties within the tetracationic cavity upon the complete oxidation of both TTF units is indicated clearly by the upfield shifts for all DNP resonances. Likewise, the TTF^{2+} units are ejected from inside the tetracationic cyclophane cavity.

8. Cyclic Voltammetry of [3]pseudorotaxane ($TTF_2 \subset 1)\cdot 4PF_6$

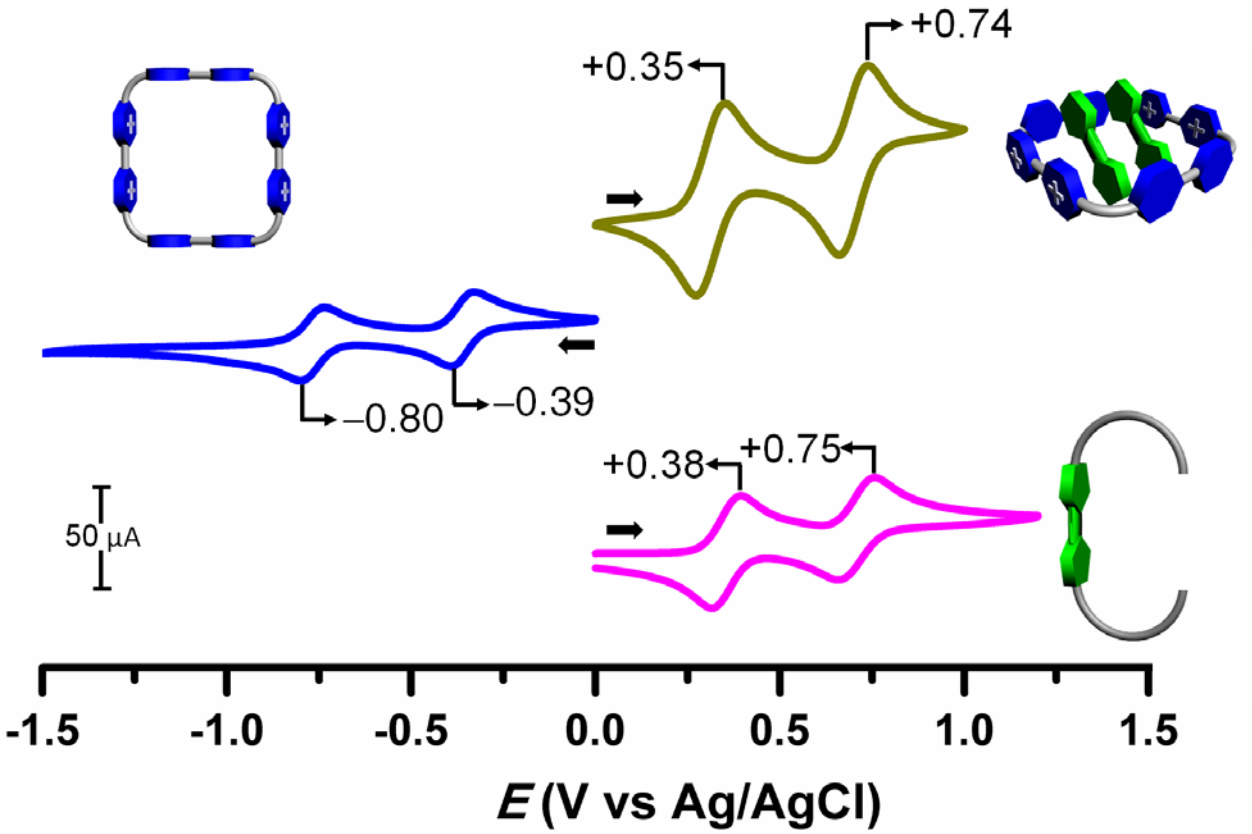

***Figure S5*:** CV spectra (1mM in MeCN, 100 mM Bu_4NPF_6, 200 mV/s) comparing (top) [3] pseudorotaxane ($TTF_2 \subset$ **1**)$\cdot 4PF_6$ with its separate constituents, (middle) **1**$\cdot 4PF_6$ and (bottom) TTF model compound **S1**. No significant shift is observed for the oxidation potential of the TTF units in the [3]pseudorotaxane (compare top and bottom spectra) which indicates that, although housed comfortably within the tetracationic cyclophane as neutral species, the TTF units quickly escape the complex upon their first oxidation to the TTF radical cation.

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9. X-Ray Structural Investigation of Possible Counterion Interactions in 3^{5+} and 3^{6+}.

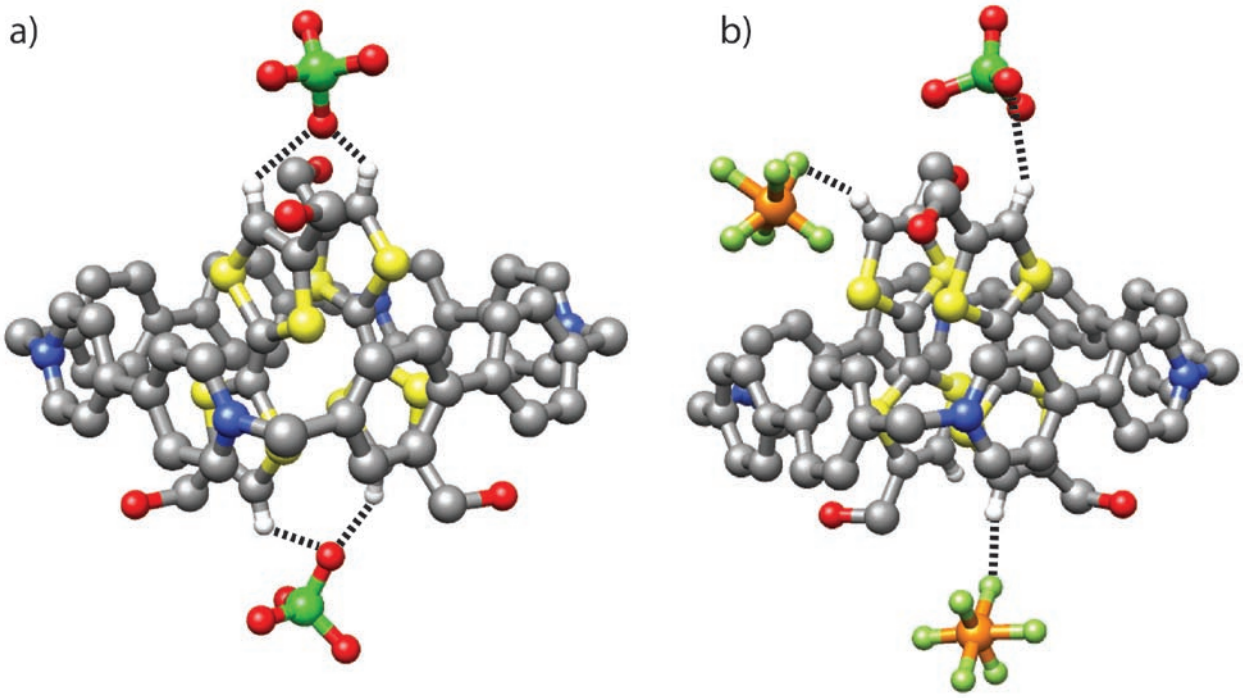

***Figure S6*:** Short contacts between counterions and oxidised TTF units in the solid-state structures of (a) **3**·4PF_6·ClO_4, with C···O distances of 2.64 and 3.12 Å, and (b) **3**·2PF_6·4ClO_4·5$MeNO_2$·$C_4H_{10}O$, with a C···O distance of 3.27 Å and C···F distances of 3.26 and 3.51 Å. Ethylene glycol chains, butadiyne units, solvent molecules, some counterions and non-TTF hydrogen atoms have been removed for clarity

10. Nanoelectrospray High Resolution MS of 3^{4+}, 3^{5+}, and 3^{6+}

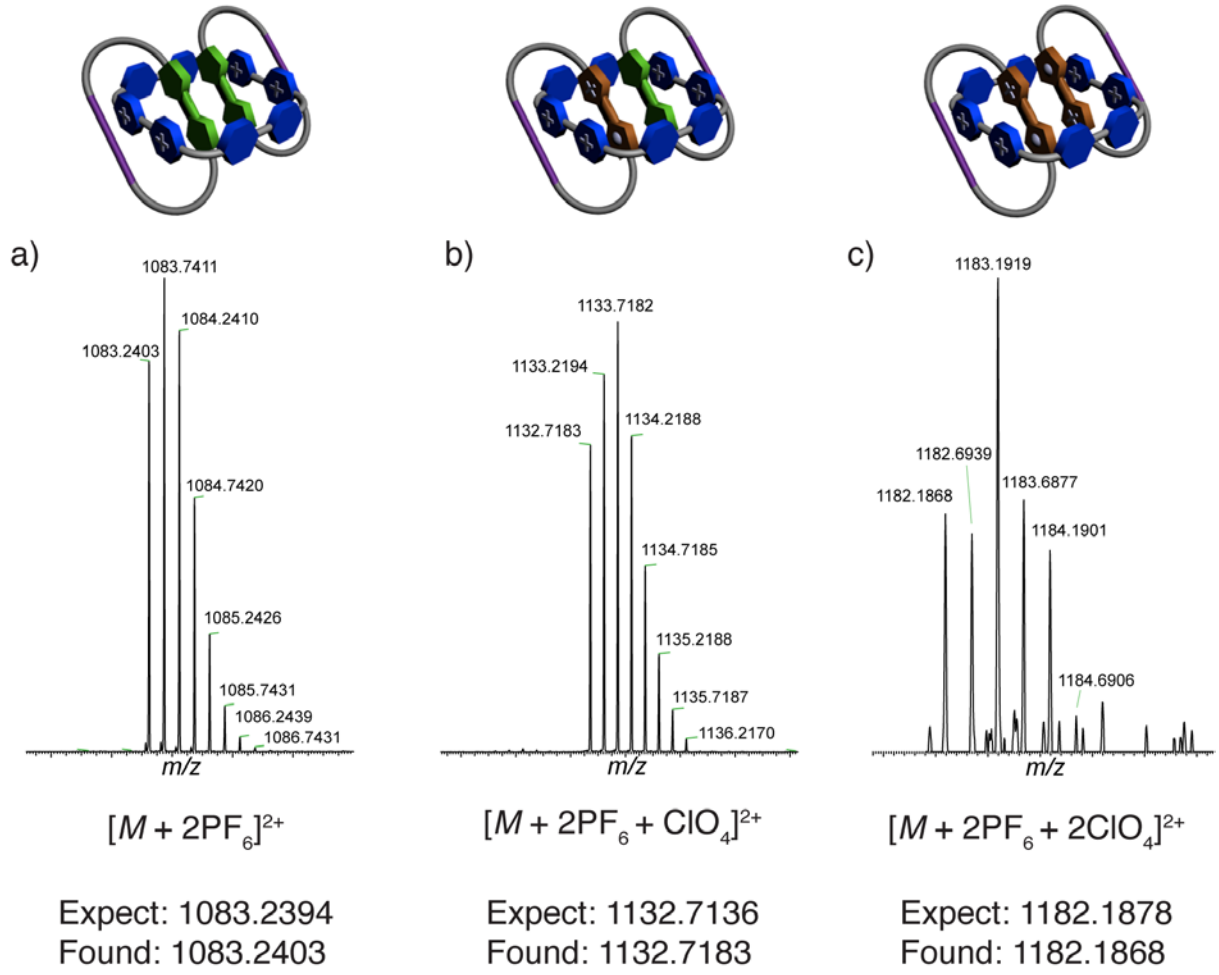

***Figure S7*:** Representative Nanoelectrospray HRMS of a) $\mathbf{3}^{4+}$, b) $\mathbf{3}^{5+}$, and c) $\mathbf{3}^{6+}$ observed for each at the 2+ ionisation state with associated PF_6^- and ClO_4^- anions. Spectra were run from a MeCN solution following the titration of 0, 1, and 2 equivalents of $Fe(ClO_4)_3$ respectively. In all cases, the lower oxidation states were also observed, usually enriched in ClO_4^- anions. These species were most likely formed through the reduction of the higher oxidised species within the reductive environment of the ionisation source for the instrument. No signals resulting from $\mathbf{3}^{7+}$ and $\mathbf{3}^{8+}$ species were observed upon introducing these highly oxidised species into the MS because they were most likely reduced to the lower oxidation states (which were observed) within the source.

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11. EPR Spectra of 3^{5+} and 7^{1+}

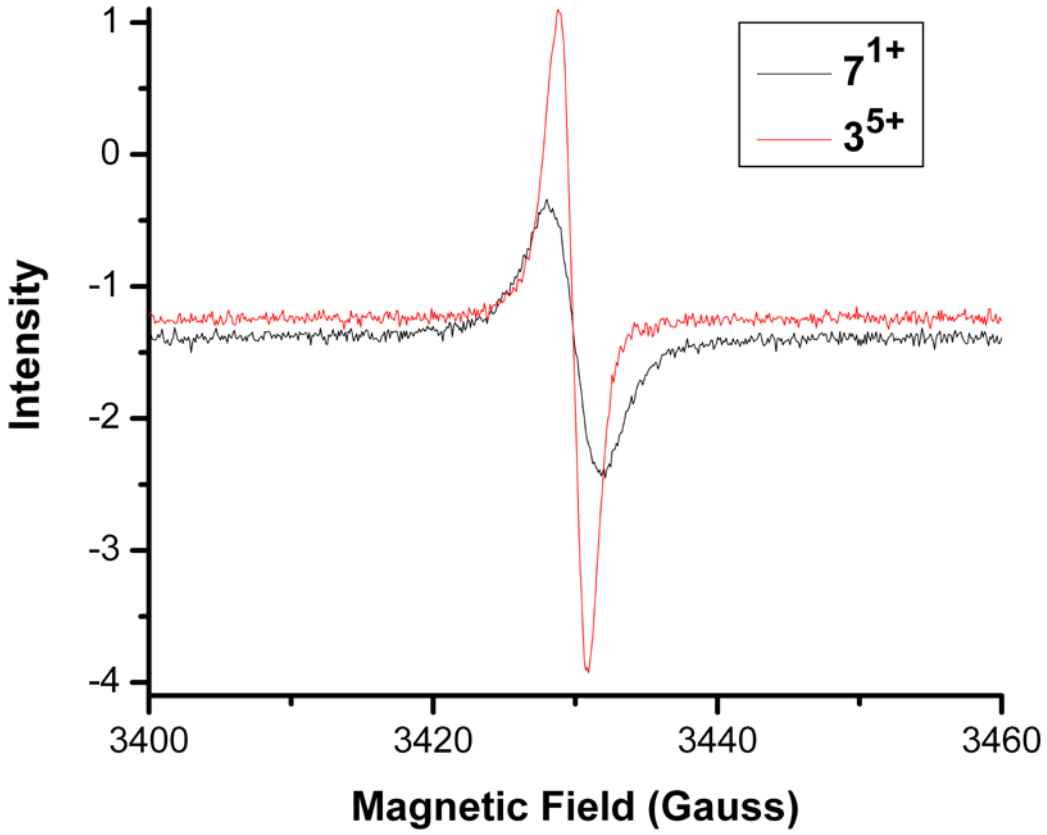

***Figure S8*:** Direct comparison of the EPR spectra of model compound $\mathbf{7}^{1+}$ (following the addition of 1 equiv of $Fe(ClO_4)_3$, displayed in black) and $\mathbf{3}^{5+}$ (following the addition of 1 equiv of $Fe(ClO_4)_3$, displayed in red). Both spectra lack hyperfine splitting but the spectrum of $\mathbf{3}^{5+}$ is more highly resolved as a consequence of sharing the radical between two TTF moieties.

12. Calculated Results

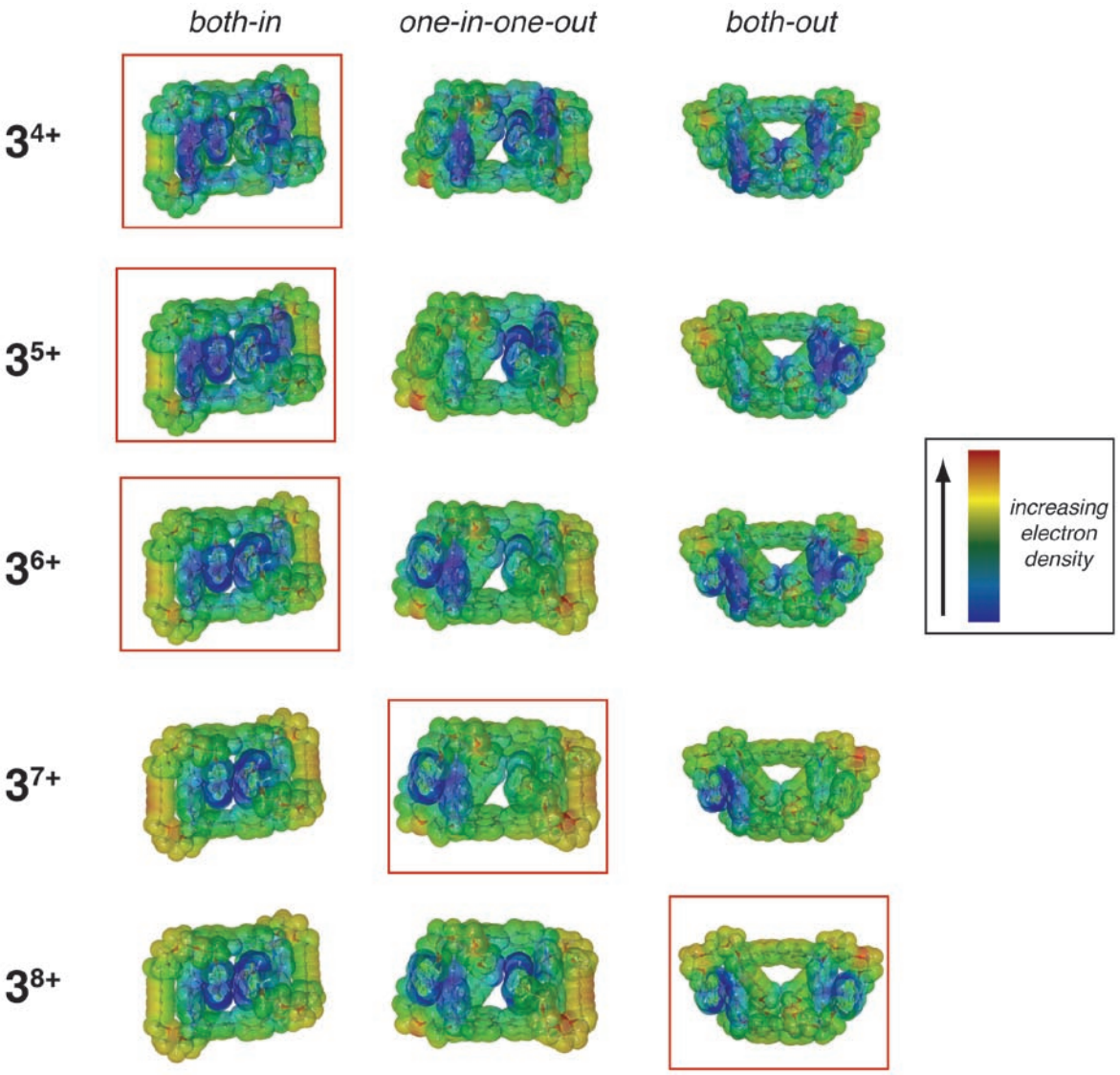

***Figure S9*:** The DFT calculated structures overlaid with the electrostatic potential maps describing the electronic interactions present across each co-conformation and oxidation state of **3**. The most stable co-conformations in all five oxidation states are framed in red.

DOI: 10.1038/NCHEM.749

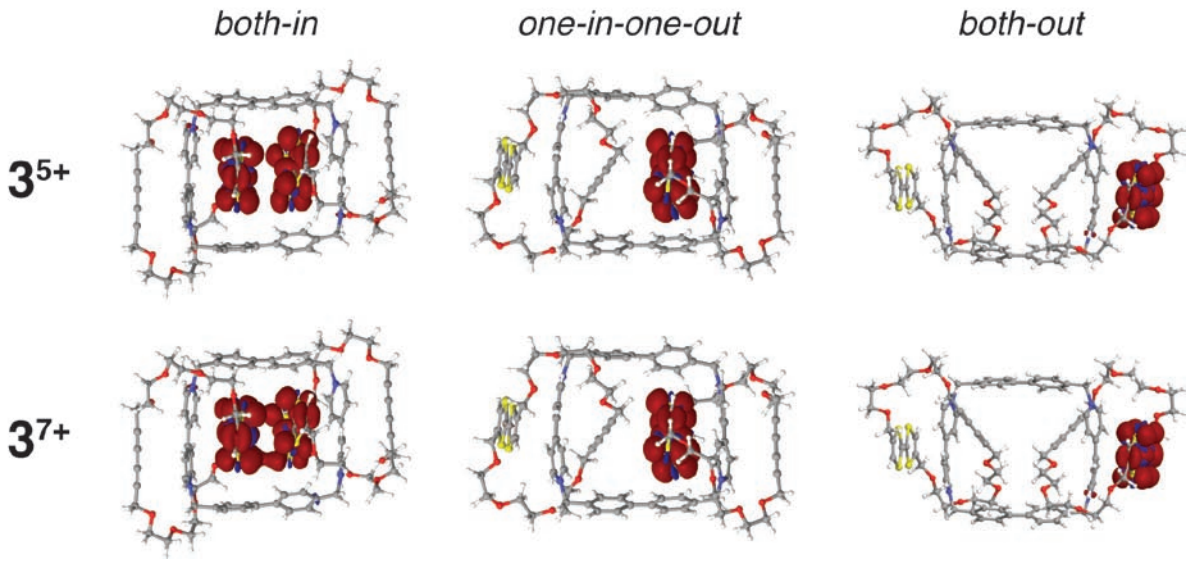

***Figure S10*:** The DFT calculated spin profiles for the co-conformations of the spin-active oxidation states, $\mathbf{3}^{5+}$ and $\mathbf{3}^{7+}$. The spin is symmetrically held on each TTF unit in the mixed-valence state of $\mathbf{3}^{5+}$ (*both-in*), while it is localised on the $TTF^{\bullet+}$ unit in the $TTF^{\bullet+}$-butadiyne interaction in the *one-in-one-out* co-conformations of $\mathbf{3}^{5+}$ and $\mathbf{3}^{7+}$.

References

S1. Asakawa, M., Ashton, P. R., Menzer, S., Raymo, F. M., Stoddart, J. F., White, A. J. P. & Williams, D. J. Cyclobis(paraquat-4,4′-biphenylene) – an organic molecular square. Chem. Eur. J. 2, 877–893 (1996).

S2. Spruell, J. M., Paxton, W. F., Olsen, J.-C., Benítez, D., Tkatchouk, E., Stern, C. L., Trabolsi, A., Friedman, D. C., Goddard, W. A. & Stoddart, J. F. A push-button molecular switch. *J. Am. Chem. Soc.* **131**, 11571–11580 (2009).

S3. Balzani, V., Credi, A., Mattersteig, G. & Williams, D. J. Switching of pseudorotaxanes and catenanes incorporating a tetrathiafulvalene unit by redox and chemical inputs. *J. Org. Chem.* **65**, 1924–1936 (2000).

S4. Amabilino, D. B., Ashton, P. R., Brown, C. L., Cordova, E., Godinez, L. A., Goodnow, T. T., Kaifer, A. E., Newton, S. P., Pietraszkiewicz, M., Philp, D., Raymo, F. M., Reder, A. S., Rutland, M. T., Slawin, A. M. Z., Spencer, N., Stoddart, J. F. & Williams, D. J. Molecular meccano 2. Self-assembly of [n]catenanes. *J. Am. Chem. Soc.* **117**, 1271–1293 (1995).

S5. Gottlieb, H. E., Kotlyar, V. & Nudelman, A. NMR chemical shifts of common laboratory solvents as trace impurities. *J. Org. Chem.* **62**, 7512–7515 (1997).

S6. Jaguar, version 7.0. Schrödinger, LLC. New York, NY (2007).

S7. Spek, A. L. Single-crystal structure validation with the program PLATON. *J. Appl. Cryst.* **36**, 7–13 (2003).

S8. Babaei, A., Connor, P. A., McQuillan, A. J. & Umapathy, S. UV-Visible spectroelectrochemistry of the reduction products of anthraquinone in dimethylformamide solutions: an advanced undergraduate experiment. *J. Chem. Ed.* **74**, 1200–1204 (1997).

Appendix: Calculated coordinates and atom-centered charge localization for the In-In, In-Out, and Out-Out co-conformations of 3.

In-in

N1	4.7192380284	2.0833270844	-3.4246041763
C2	3.9857067619	2.0091663448	-2.2935327541
C3	4.6033486747	1.7882118312	-1.0798672489
C4	5.9946073574	1.6517118938	-0.9914068620
C5	6.7174602361	1.7242341292	-2.1963271400
C6	6.0622013068	1.9359477010	-3.3816326278
C7	6.6731527439	1.5085468095	0.2941305668
C8	6.0140860813	0.9846244213	1.4202034228
C9	6.6385511887	0.9632480884	2.6445334262
N10	7.8870199837	1.4553581985	2.7957147132
C11	8.5748342346	1.9128248346	1.7279066045
C12	7.9978338867	1.9369707274	0.4777861287
C13	8.4419648738	1.7064260645	4.1563477172
C14	8.0655840895	3.1057401364	4.5505854532
C15	6.8226205063	3.3578560687	5.1348847705
C16	6.3873897866	4.6578270195	5.3438626490
C17	7.1889547774	5.7503574254	4.9901340226
C18	8.4670410627	5.4871050847	4.4786591198
C19	8.8944126830	4.1864782502	4.2395552522
C20	4.8975146022	6.7555203544	-4.9585320061
C21	3.7982849066	6.2636569116	-4.2381815839
C22	3.5107532215	4.9073689269	-4.1967864658
C23	4.3151955754	3.9912523147	-4.8770926479
C24	5.4035161387	4.4720662231	-5.6099251616
C25	5.6922913847	5.8322939535	-5.6501082887
C26	4.0873790442	2.5186720818	-4.6998264733
H27	2.9064181674	2.1237249731	-2.4028546495
H28	3.9797867344	1.7763853537	-0.1879042074
H29	7.7938775673	1.5810242005	-2.2159149188
H30	6.5760592678	2.0007461815	-4.3361804918
H31	5.0168642992	0.5603737804	1.3397090397
H32	6.1703273364	0.5694118794	3.5419081809
H33	9.5761143170	2.2855053429	1.9339071733
H34	8.5813322990	2.3637627179	-0.3346693281
H35	8.0187483484	0.9421417355	4.8137273288
H36	9.5199879207	1.5244928142	4.0817122982
H37	6.1789600032	2.5256986707	5.4219563500
H38	5.4159414403	4.8306822271	5.8022521869
H39	9.1148310746	6.3197715802	4.2024821851
H40	9.8674137919	4.0022163070	3.7789969291
H41	3.1754935380	6.9553973397	-3.6731849376
H42	2.6652613070	4.5502630348	-3.6061251879
H43	6.0250471039	3.7779966295	-6.1762649391
H44	6.5254742137	6.1853085868	-6.2559260064
H45	3.0295893079	2.2522685193	-4.6228266372
H46	4.5256193047	1.9134053755	-5.4991865701
O47	1.3157285394	4.0154508811	-1.4242170632
C48	0.0781090462	3.7590398651	-2.0857744039
C49	-0.1804793170	2.2869608324	-2.2779732554
O50	0.8101816402	1.7656727204	-3.1402441003
C51	0.5382445604	0.4116747368	-3.4837494850
C52	1.5542463872	-0.0429946160	-4.4994511961
O53	2.8489334184	-0.2040898856	-3.9385489742
C54	3.0653408091	-1.5136508081	-3.4260787007
C55	4.0644563226	-1.4569611775	-2.3001613110
O56	5.3006621335	-0.9338824400	-2.7752563121
C57	6.4150693714	-1.7942625310	-2.5895672352
C58	9.0449845571	-2.3950093856	3.5336997312
O59	9.3705447634	-1.1685261160	4.1718252955
C60	10.2903681092	-1.3927243744	5.2356809150
C61	10.7197322550	-0.0721005003	5.8146413441
O62	11.3904545175	0.6502528482	4.8021929094
C63	11.7662643757	1.9475595449	5.2018840429
C64	12.4826299872	2.5876911724	4.0434289912

DOI: 10.1038/NCHEM.749

O65	11.6320978358	2.5722537878	2.8977410857
C66	12.3137612274	2.8718756711	1.6909324826
C67	11.9854470606	4.2450548094	1.1636379543
O68	10.6445138569	4.2226864063	0.6739908775
C69	10.3464764519	5.3685294509	-0.0893246170
C70	8.8969997319	5.3366109769	-0.4363806076
C71	8.3659703647	5.3914440021	-1.6715746365
S72	6.6341822029	5.3518449221	-1.8548175894
C73	6.3485273777	5.1507898064	-0.1222459066
S74	7.7694743468	5.2194786227	0.9045226579
C75	5.0977672977	4.9265759370	0.3757057743
S76	4.7809185137	4.4772480418	2.0504219513
C77	3.1145726201	4.0474071316	1.7274845344
C78	2.6179138977	4.2522833824	0.4953923311
S79	3.6966412184	4.9997030636	-0.6719465217
C80	1.2435308978	3.9414716977	-0.0174715343
H81	0.1627858773	4.2445724686	-3.0630159422
H82	-0.7531750675	4.2274567181	-1.5383051436
H83	-0.1765373073	1.7469424431	-1.3133272998
H84	-1.1843691700	2.1489484732	-2.7134658348
H85	-0.4769274712	0.3329139300	-3.9059683809
H86	0.5689778529	-0.2260886189	-2.5823107234
H87	1.2139227591	-0.9700170877	-4.9829795831
H88	1.6392690265	0.7141474830	-5.2887682418
H89	3.4381013574	-2.1671158307	-4.2295702624
H90	2.1263791650	-1.9469078770	-3.0453984374
H91	3.6934748432	-0.8026690699	-1.4940227270
H92	4.1961319464	-2.4618225689	-1.8757971341
H93	7.1995170056	-1.4053320452	-3.2521667060
H94	6.1856692820	-2.8121982552	-2.9468625477
H95	8.4052234111	-3.0169027258	4.1856342095
H96	9.9624761967	-2.9843552403	3.3546700490
H97	11.1744585795	-1.9287034296	4.8544206661
H98	9.8348511094	-2.0150266237	6.0236020437
H99	9.8481835457	0.4997245111	6.1858837942
H100	11.3803470610	-0.2479609949	6.6796857306
H101	12.4406334059	1.9256842462	6.0752194265
H102	10.8758515152	2.5357844243	5.5004069124
H103	12.7771287465	3.6179997785	4.3059409542
H104	13.3972825778	2.0179678598	3.8235177933
H105	12.0144007952	2.1240913710	0.9429895189
H106	13.4003089719	2.7803208776	1.8274963022
H107	12.0874919168	5.0172169713	1.9458132320
H108	12.6767609736	4.4999094117	0.3436616833
H109	10.9481167177	5.4005448461	-1.0144159953
H110	10.5852220268	6.2854944994	0.4864375521
H111	8.9593156657	5.4758146583	-2.5778329291
H112	2.5450499745	3.6274251115	2.5512019991
H113	0.9247813946	2.9435775463	0.3296394635
H114	0.5027506740	4.6664689508	0.3632967339
C115	8.3952120229	-2.1621012402	2.2583983441
C116	7.8880845930	-2.0532696381	1.1563402350
C117	7.3545218458	-1.9417838022	-0.0900215216
C118	6.9011536089	-1.8538136889	-1.2181628605
N119	5.2972225796	11.6933336688	3.9290081783
C120	4.2075271038	11.6391262325	3.1341871356
C121	4.3122412338	11.9320431807	1.7910398654
C122	5.5449856977	12.2739866092	1.2216547096
C123	6.6504809911	12.3346591938	2.0889657465
C124	6.4986371915	12.0449890368	3.4206351157
C125	5.6919915727	12.4858059052	-0.2158321601
C126	4.6079356814	12.8801991383	-1.0202797404
C127	4.7444724910	12.9514571384	-2.3860091007
N128	5.9128657861	12.6312402985	-2.9830576033
C129	6.9914723024	12.3060850385	-2.2411651128
C130	6.9105104106	12.2445836075	-0.8688521193
C131	5.9849281801	12.4200431393	-4.4564519579
C132	5.7299301340	10.9639223013	-4.7339662160
C133	4.4179293940	10.4928558063	-4.8143167945
C134	4.1590355561	9.1341785546	-4.9060114921
C135	5.2025614078	8.1986114896	-4.9408504802
C136	6.5192787846	8.6809653916	-4.9183352354

C137	6.7804489310	10.0430059286	-4.7983991680
C138	6.6883727530	7.1298372540	5.1136761959
C139	5.3257475864	7.4158175808	4.9402822654
C140	4.8471885468	8.7145460312	5.0490788253
C141	5.7104017382	9.7658644536	5.3601086161
C142	7.0631250393	9.4840054361	5.5676158332
C143	7.5429228368	8.1858681130	5.4575306646
C144	5.2256015169	11.1851141989	5.3269647614
H145	3.2701633804	11.3609557186	3.6158264547
H146	3.4188713313	11.8348930859	1.1775525788
H147	7.6296761224	12.6404851201	1.7321484527
H148	7.3212014902	12.0787572828	4.1284252237
H149	3.6561448568	13.1637366602	-0.5799734443
H150	3.9375423466	13.2535615110	-3.0469441116
H151	7.8917722438	12.0609752854	-2.7982264086
H152	7.7989249293	11.9254675118	-0.3289668775
H153	5.2340309494	13.0799042978	-4.9005301254
H154	6.9752212024	12.7761624724	-4.7611551310
H155	3.5849344954	11.1972822579	-4.7999755140
H156	3.1293102581	8.7886279448	-4.9824299020
H157	7.3501485491	7.9737252976	-4.9247926775
H158	7.8087957678	10.4020764661	-4.7208846318
H159	4.6439761636	6.6212536821	4.6407919523
H160	3.7930609837	8.9218379425	4.8594823844
H161	7.7485217757	10.2847679854	5.8459593202
H162	8.5980785136	7.9876836267	5.6381874618
H163	4.1831220683	11.2942240907	5.6368358651
H164	5.8300560081	11.8585613969	5.9423756405
O165	1.8448035874	9.1835662148	3.2501127390
C166	0.9046460978	9.2495999046	4.3232234289
C167	0.4693913701	10.6580125555	4.6339353980
O168	1.5882278198	11.3806143424	5.1001049204
C169	1.2205691535	12.6787730028	5.5512186924
C170	2.4318168787	13.3444661111	6.1479155326
O171	3.3888987515	13.7025121792	5.1613453369
C172	3.1789029535	15.0104245741	4.6410814035
C173	3.6979105770	15.0805143118	3.2282307658
O174	5.0908470200	14.7881713232	3.2068660278
C175	5.8981949035	15.8216951316	2.6606096866
C176	5.9809628959	16.6141357720	-3.9854195066
O177	6.2693942470	15.4400063625	-4.7309245474
C178	6.6767369751	15.7860296910	-6.0515360529
C179	7.1023259737	14.5443422067	-6.7865958693
O180	8.2237992553	14.0029688170	-6.1183629877
C181	8.6556878600	12.7751457671	-6.6563566017
C182	9.8445437779	12.3142470954	-5.8538897246
O183	9.4730115148	12.2124583632	-4.4783635295
C184	10.5801660997	12.0863819615	-3.6004686159
C185	10.7182664658	10.6956206984	-3.0309114216
O186	9.6630024394	10.4929791826	-2.0892478300
C187	9.8729906327	9.3475298425	-1.2943482188
C188	8.6624349972	9.1273884158	-0.4512955796
C189	8.6261544353	9.0144800348	0.8906549136
S190	7.0996499084	8.7344566964	1.6830892733
C191	6.1829399811	8.8326984878	0.1738228542
S192	7.1309835299	8.9886359554	-1.2956870313
C193	4.8197515969	8.8209275346	0.1669986384
S194	3.8443697663	9.1355580774	-1.2667597859
C195	2.3625570721	9.2997748304	-0.3446297219
C196	2.3886438503	9.0663594488	0.9792784511
S197	3.9259874452	8.5477937819	1.6500802118
C198	1.2612627487	9.1644600010	1.9662364813
H199	1.4213468579	8.8312194997	5.1922446744
H200	0.0327986674	8.6170149510	4.1066156958
H201	0.0341379493	11.1508602424	3.7454336532
H202	-0.3212556226	10.6311021143	5.4029328153
H203	0.4224513940	12.5956352113	6.3072493698
H204	0.8176283049	13.2740829724	4.7124145065
H205	2.1274531786	14.2170736595	6.7420603291
H206	2.9223011041	12.6476696635	6.8387395521
H207	3.6984089748	15.7461015807	5.2728505218
H208	2.1076098557	15.2650271482	4.6383574784

DOI: 10.1038/NCHEM.749

H209	3.1756473693	14.3467030079	2.5941066997
H210	3.4958155305	16.0769156605	2.8111158248
H211	6.9228207026	15.5955536394	2.9837108505
H212	5.6407645691	16.7962879295	3.1068568398
H213	5.0443091307	17.0820159103	-4.3394510487
H214	6.7751902795	17.3666452805	-4.1416542397
H215	7.5234306635	16.4899534045	-6.0064082720
H216	5.8566907449	16.2815934952	-6.5973875558
H217	6.2797779468	13.8047914469	-6.8221670887
H218	7.3494199048	14.8011192733	-7.8302895488
H219	8.9536333110	12.8751335560	-7.7144418059
H220	7.8341644973	12.0313384780	-6.6243595215
H221	10.2062706067	11.3450399950	-6.2392418722
H222	10.6586720013	13.0467363961	-5.9557462633
H223	10.4343326812	12.7955967616	-2.7724276453
H224	11.5117085870	12.3667671692	-4.1119165989
H225	10.6696652889	9.9262296959	-3.8217787131
H226	11.6919158341	10.5990485681	-2.5235894566
H227	10.7584338505	9.4666827398	-0.6468881486
H228	10.0571775420	8.4648118385	-1.9399895492
H229	9.5078345413	9.0653900701	1.5221987222
H230	1.4720020141	9.5876545649	-0.8934511826
H231	0.6626476333	10.0697682231	1.7707306472
H232	0.5784996696	8.3022442633	1.8751928335
C233	5.8959715085	16.3258622333	-2.5666313213
C234	5.8490039756	16.1814097754	-1.3577444928
C235	5.8324417044	16.0349168180	-0.0050921676
C236	5.8395277059	15.9153667229	1.2083544232

4^{+}

Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.20299	0.33113	-0.23540	0.13500	-0.23332
Atom	C6	C7	C8	C9	N10
Charge	-0.02338	0.16361	-0.17086	-0.18115	-0.03285
Atom	C11	C12	C13	C14	C15
Charge	0.21829	-0.15819	-0.00219	0.07216	-0.35270
Atom	C16	C17	C18	C19	C20
Charge	-0.04370	0.07456	-0.30997	-0.00853	-0.16032
Atom	C21	C22	C23	C24	C25
Charge	-0.11406	-0.15370	0.14258	-0.40464	0.10348
Atom	C26	H27	H28	H29	H30
Charge	-0.13039	0.15676	0.12721	0.23060	0.24380
Atom	H31	H32	H33	H34	H35
Charge	0.22188	0.27577	0.04509	0.10305	0.15066
Atom	H36	H37	H38	H39	H40
Charge	0.00624	0.21316	0.16017	0.19868	0.15010
Atom	H41	H42	H43	H44	H45
Charge	0.15423	0.11118	0.21509	0.11376	0.11870
Atom	H46	O47	C48	C49	O50
Charge	0.19555	-0.19939	-0.10132	-0.03174	-0.29651
Atom	C51	C52	O53	C54	C55
Charge	-0.06049	0.02051	-0.37938	-0.00565	-0.02645
Atom	O56	C57	C58	O59	C60
Charge	-0.23826	-0.18422	-0.16119	-0.17592	-0.15505
Atom	C61	O62	C63	C64	O65

Charge	0.08726	-0.39778	0.11733	-0.18012	-0.23891
Atom	C66	C67	O68	C69	C70
Charge	-0.01592	-0.08245	-0.21261	-0.20429	0.24830
Atom	C71	S72	C73	S74	C75
Charge	-0.42585	0.15947	-0.13211	-0.03749	-0.02906
Atom	S76	C77	C78	S79	C80
Charge	0.13910	-0.42672	0.17787	-0.10993	-0.13743
Atom	H81	H82	H83	H84	H85
Charge	0.12830	0.12698	0.08928	0.12069	0.11035
Atom	H86	H87	H88	H89	H90
Charge	0.10525	0.10029	0.10229	0.10377	0.10565
Atom	H91	H92	H93	H94	H95
Charge	0.08323	0.11376	0.18305	0.19882	0.17288
Atom	H96	H97	H98	H99	H100
Charge	0.17304	0.14152	0.12364	0.06572	0.10194
Atom	H101	H102	H103	H104	H105
Charge	0.10753	-0.00623	0.13287	0.15234	0.09590
Atom	H106	H107	H108	H109	H110
Charge	0.11246	0.11317	0.12526	0.13840	0.12025
Atom	H111	H112	H113	H114	C115
Charge	0.26581	0.28943	0.13938	0.14375	0.02310
Atom	C116	C117	C118	N119	C120
Charge	-0.08684	-0.13469	0.00919	-0.18354	0.29609
Atom	C121	C122	C123	C124	C125
Charge	-0.25259	0.11484	-0.21700	-0.04753	0.15116
Atom	C126	C127	N128	C129	C130
Charge	-0.13901	-0.19831	0.00186	0.16757	-0.12972
Atom	C131	C132	C133	C134	C135
Charge	-0.05698	0.13808	-0.39616	0.01789	-0.02510
Atom	C136	C137	C138	C139	C140
Charge	-0.20247	-0.11103	-0.20712	-0.07985	-0.13899
Atom	C141	C142	C143	C144	H145
Charge	0.12075	-0.36475	0.07565	-0.14061	0.17478
Atom	H146	H147	H148	H149	H150
Charge	0.14339	0.23211	0.25514	0.22021	0.27680
Atom	H151	H152	H153	H154	H155
Charge	0.05966	0.09208	0.15901	0.03051	0.22135
Atom	H156	H157	H158	H159	H160
Charge	0.15096	0.18102	0.17261	0.13746	0.09807
Atom	H161	H162	H163	H164	O165
Charge	0.20518	0.12437	0.12741	0.19821	-0.18562
Atom	C166	C167	O168	C169	C170
Charge	-0.09905	-0.05307	-0.28908	-0.06683	0.03884
Atom	O171	C172	C173	O174	C175
Charge	-0.38849	-0.01388	-0.03021	-0.22261	-0.20361
Atom	C176	O177	C178	C179	O180
Charge	-0.16302	-0.17200	-0.16829	0.09096	-0.39680
Atom	C181	C182	O183	C184	C185

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Charge	0.09811	-0.16350	-0.25200	-0.00397	-0.10015
Atom	O186	C187	C188	C189	S190
Charge	-0.19804	-0.16498	0.20033	-0.42252	0.12299
Atom	C191	S192	C193	S194	C195
Charge	0.06391	-0.09888	-0.02993	0.11169	-0.42325
Atom	C196	S197	C198	H199	H200
Charge	0.15543	-0.12018	-0.13874	0.12819	0.12640
Atom	H201	H202	H203	H204	H205
Charge	0.09606	0.12576	0.10978	0.10635	0.09738
Atom	H206	H207	H208	H209	H210
Charge	0.09599	0.10579	0.10807	0.09136	0.11224
Atom	H211	H212	H213	H214	H215
Charge	0.18592	0.20092	0.17275	0.17369	0.14481
Atom	H216	H217	H218	H219	H220
Charge	0.12703	0.06451	0.10143	0.11066	0.00048
Atom	H221	H222	H223	H224	H225
Charge	0.12836	0.15105	0.09316	0.11158	0.11804
Atom	H226	H227	H228	H229	H230
Charge	0.12623	0.12728	0.11921	0.26737	0.28885
Atom	H231	H232	C233	C234	C235
Charge	0.14370	0.14330	0.01386	-0.06741	-0.15757
Atom	C236				
Charge	0.03107				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.22718	0.36015	-0.21485	0.10339	-0.23210
Atom	C6	C7	C8	C9	N10
Charge	0.01854	0.19315	-0.17454	-0.14702	-0.07377
Atom	C11	C12	C13	C14	C15
Charge	0.25737	-0.18070	0.01314	0.08942	-0.37160
Atom	C16	C17	C18	C19	C20
Charge	0.00829	0.00939	-0.26034	-0.03056	-0.10317
Atom	C21	C22	C23	C24	C25
Charge	-0.15546	-0.12759	0.14436	-0.40147	0.09521
Atom	C26	H27	H28	H29	H30
Charge	-0.12337	0.13497	0.12205	0.23400	0.23772
Atom	H31	H32	H33	H34	H35
Charge	0.22241	0.27468	0.03359	0.10980	0.15918
Atom	H36	H37	H38	H39	H40
Charge	0.01288	0.21637	0.15266	0.18712	0.14907
Atom	H41	H42	H43	H44	H45
Charge	0.15855	0.10367	0.22181	0.12244	0.11991
Atom	H46	O47	C48	C49	O50
Charge	0.20467	-0.21150	-0.11949	-0.02452	-0.29557
Atom	C51	C52	O53	C54	C55

Charge	-0.06261	0.01853	-0.38180	-0.00117	-0.02875
Atom	O56	C57	C58	O59	C60
Charge	-0.24627	-0.17925	-0.16026	-0.18316	-0.16132
Atom	C61	O62	C63	C64	O65
Charge	0.09594	-0.39729	0.10582	-0.16981	-0.24496
Atom	C66	C67	O68	C69	C70
Charge	-0.01570	-0.09744	-0.20703	-0.19703	0.23222
Atom	C71	S72	C73	S74	C75
Charge	-0.36377	0.20629	-0.14379	0.02360	-0.05704
Atom	S76	C77	C78	S79	C80
Charge	0.21517	-0.37067	0.14504	-0.00105	-0.11672
Atom	H81	H82	H83	H84	H85
Charge	0.14008	0.13792	0.08739	0.12797	0.11428
Atom	H86	H87	H88	H89	H90
Charge	0.10711	0.10470	0.10420	0.10597	0.10744
Atom	H91	H92	H93	H94	H95
Charge	0.07831	0.11865	0.18260	0.20294	0.17509
Atom	H96	H97	H98	H99	H100
Charge	0.17629	0.14436	0.12741	0.06000	0.10371
Atom	H101	H102	H103	H104	H105
Charge	0.11223	-0.00238	0.13193	0.15452	0.09817
Atom	H106	H107	H108	H109	H110
Charge	0.11929	0.12106	0.13725	0.15629	0.12521
Atom	H111	H112	H113	H114	C115
Charge	0.28266	0.30453	0.15599	0.15288	0.02755
Atom	C116	C117	C118	N119	C120
Charge	-0.09200	-0.12853	0.00378	-0.20740	0.31722
Atom	C121	C122	C123	C124	C125
Charge	-0.22905	0.10670	-0.22182	-0.00483	0.15696
Atom	C126	C127	N128	C129	C130
Charge	-0.14196	-0.16304	-0.03081	0.19533	-0.14080
Atom	C131	C132	C133	C134	C135
Charge	-0.03464	0.14034	-0.39905	0.05668	-0.09168
Atom	C136	C137	C138	C139	C140
Charge	-0.15762	-0.12064	-0.17156	-0.11037	-0.12835
Atom	C141	C142	C143	C144	H145
Charge	0.13816	-0.37514	0.08708	-0.14260	0.15880
Atom	H146	H147	H148	H149	H150
Charge	0.13946	0.23382	0.24737	0.22103	0.27482
Atom	H151	H152	H153	H154	H155
Charge	0.04847	0.09602	0.16343	0.03340	0.22202
Atom	H156	H157	H158	H159	H160
Charge	0.14838	0.16757	0.17019	0.14252	0.09571
Atom	H161	H162	H163	H164	O165
Charge	0.21395	0.12772	0.13013	0.20720	-0.19415
Atom	C166	C167	O168	C169	C170
Charge	-0.11713	-0.04204	-0.28952	-0.06939	0.03614
Atom	O171	C172	C173	O174	C175

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Charge	-0.38840	-0.01154	-0.02596	-0.23611	-0.19200
Atom	C176	O177	C178	C179	O180
Charge	-0.16186	-0.17952	-0.16967	0.09765	-0.39631
Atom	C181	C182	O183	C184	C185
Charge	0.08950	-0.15701	-0.25521	-0.00364	-0.11772
Atom	O186	C187	C188	C189	S190
Charge	-0.18371	-0.16652	0.16677	-0.34756	0.12964
Atom	C191	S192	C193	S194	C195
Charge	0.05805	-0.06786	-0.05021	0.14864	-0.36051
Atom	C196	S197	C198	H199	H200
Charge	0.10809	-0.05904	-0.12302	0.13610	0.13455
Atom	H201	H202	H203	H204	H205
Charge	0.09492	0.12986	0.11284	0.10901	0.10133
Atom	H206	H207	H208	H209	H210
Charge	0.09703	0.10719	0.10940	0.08524	0.11561
Atom	H211	H212	H213	H214	H215
Charge	0.18377	0.20271	0.17467	0.17619	0.14600
Atom	H216	H217	H218	H219	H220
Charge	0.12921	0.06021	0.10229	0.11465	0.00275
Atom	H221	H222	H223	H224	H225
Charge	0.12761	0.15302	0.09447	0.11769	0.12602
Atom	H226	H227	H228	H229	H230
Charge	0.13636	0.14083	0.12650	0.27107	0.29879
Atom	H231	H232	C233	C234	C235
Charge	0.16018	0.14904	0.01719	-0.07319	-0.14785
Atom	C236				
Charge	0.02097				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.24285	0.38261	-0.20674	0.08969	-0.23840
Atom	C6	C7	C8	C9	N10
Charge	0.05054	0.20965	-0.17742	-0.12006	-0.10416
Atom	C11	C12	C13	C14	C15
Charge	0.28532	-0.19722	0.01961	0.10916	-0.38372
Atom	C16	C17	C18	C19	C20
Charge	0.04998	-0.05344	-0.21157	-0.05332	-0.05965
Atom	C21	C22	C23	C24	C25
Charge	-0.19054	-0.10513	0.15390	-0.40271	0.09417
Atom	C26	H27	H28	H29	H30
Charge	-0.12311	0.11973	0.12092	0.23729	0.23270
Atom	H31	H32	H33	H34	H35
Charge	0.22176	0.27313	0.02507	0.11523	0.16654
Atom	H36	H37	H38	H39	H40
Charge	0.01968	0.21859	0.14900	0.17448	0.14882

Atom	H41	H42	H43	H44	H45
Charge	0.16446	0.09556	0.22848	0.12990	0.12164
Atom	H46	O47	C48	C49	O50
Charge	0.21257	-0.21625	-0.13574	-0.01483	-0.29542
Atom	C51	C52	O53	C54	C55
Charge	-0.06713	0.01964	-0.38479	0.00173	-0.02952
Atom	O56	C57	C58	O59	C60
Charge	-0.25307	-0.17460	-0.15837	-0.18923	-0.16593
Atom	C61	O62	C63	C64	O65
Charge	0.10381	-0.39694	0.09687	-0.15959	-0.25072
Atom	C66	C67	O68	C69	C70
Charge	-0.01326	-0.11592	-0.19510	-0.18319	0.18463
Atom	C71	S72	C73	S74	C75
Charge	-0.27705	0.20388	-0.13458	0.05285	-0.07736
Atom	S76	C77	C78	S79	C80
Charge	0.24440	-0.30428	0.10652	0.06349	-0.10776
Atom	H81	H82	H83	H84	H85
Charge	0.14939	0.14631	0.08499	0.13312	0.11809
Atom	H86	H87	H88	H89	H90
Charge	0.10933	0.10790	0.10511	0.10811	0.10882
Atom	H91	H92	H93	H94	H95
Charge	0.07360	0.12251	0.18215	0.20576	0.17630
Atom	H96	H97	H98	H99	H100
Charge	0.17902	0.14674	0.13016	0.05476	0.10494
Atom	H101	H102	H103	H104	H105
Charge	0.11585	0.00039	0.13004	0.15619	0.09990
Atom	H106	H107	H108	H109	H110
Charge	0.12514	0.12822	0.14766	0.16880	0.12524
Atom	H111	H112	H113	H114	C115
Charge	0.28723	0.31124	0.17256	0.16123	0.03084
Atom	C116	C117	C118	N119	C120
Charge	-0.09559	-0.12499	0.00078	-0.24323	0.34447
Atom	C121	C122	C123	C124	C125
Charge	-0.20745	0.09647	-0.23286	0.04558	0.16339
Atom	C126	C127	N128	C129	C130
Charge	-0.14760	-0.12610	-0.07389	0.23209	-0.15159
Atom	C131	C132	C133	C134	C135
Charge	-0.00354	0.13821	-0.40631	0.10632	-0.15651
Atom	C136	C137	C138	C139	C140
Charge	-0.11169	-0.12995	-0.13296	-0.13677	-0.12022
Atom	C141	C142	C143	C144	H145
Charge	0.15397	-0.38528	0.10004	-0.14001	0.13817
Atom	H146	H147	H148	H149	H150
Charge	0.13373	0.23810	0.23925	0.22383	0.27332
Atom	H151	H152	H153	H154	H155
Charge	0.03228	0.09832	0.16863	0.03765	0.22262
Atom	H156	H157	H158	H159	H160
Charge	0.14146	0.15513	0.16606	0.14296	0.09564

DOI: 10.1038/NCHEM.749

Atom	H161	H162	H163	H164	O165
Charge	0.22260	0.13016	0.13203	0.21737	-0.21146
Atom	C166	C167	O168	C169	C170
Charge	-0.13184	-0.03547	-0.28952	-0.06863	0.03098
Atom	O171	C172	C173	O174	C175
Charge	-0.38749	-0.00744	-0.02619	-0.24510	-0.18603
Atom	C176	O177	C178	C179	O180
Charge	-0.15954	-0.18787	-0.17460	0.10646	-0.39613
Atom	C181	C182	O183	C184	C185
Charge	0.07810	-0.14802	-0.25895	-0.00542	-0.13069
Atom	O186	C187	C188	C189	S190
Charge	-0.17552	-0.17087	0.16173	-0.27745	0.17039
Atom	C191	S192	C193	S194	C195
Charge	0.04414	-0.00725	-0.08077	0.22864	-0.29998
Atom	C196	S197	C198	H199	H200
Charge	0.08012	0.04596	-0.10241	0.14583	0.14442
Atom	H201	H202	H203	H204	H205
Charge	0.09496	0.13639	0.11611	0.11060	0.10609
Atom	H206	H207	H208	H209	H210
Charge	0.09887	0.10870	0.11070	0.07982	0.12011
Atom	H211	H212	H213	H214	H215
Charge	0.18281	0.20604	0.17647	0.17892	0.14852
Atom	H216	H217	H218	H219	H220
Charge	0.13242	0.05448	0.10349	0.11932	0.00651
Atom	H221	H222	H223	H224	H225
Charge	0.12651	0.15565	0.09734	0.12464	0.13424
Atom	H226	H227	H228	H229	H230
Charge	0.14764	0.15834	0.13716	0.28348	0.31707
Atom	H231	H232	C233	C234	C235
Charge	0.17881	0.15907	0.02168	-0.07830	-0.14178
Atom	C236				
Charge	0.01598				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.25784	0.36913	-0.20774	0.09458	-0.25610
Atom	C6	C7	C8	C9	N10
Charge	0.06460	0.21261	-0.18333	-0.09448	-0.12725
Atom	C11	C12	C13	C14	C15
Charge	0.30083	-0.20433	-0.00300	0.14024	-0.38302
Atom	C16	C17	C18	C19	C20
Charge	0.07697	-0.12763	-0.14353	-0.10229	-0.01689
Atom	C21	C22	C23	C24	C25
Charge	-0.22833	-0.07881	0.15860	-0.39320	0.07951
Atom	C26	H27	H28	H29	H30
Charge	-0.12444	0.13075	0.12783	0.24383	0.23401

Atom	H31	H32	H33	H34	H35
Charge	0.22145	0.27163	0.02115	0.11925	0.17716
Atom	H36	H37	H38	H39	H40
Charge	0.03805	0.21961	0.14932	0.15698	0.15504
Atom	H41	H42	H43	H44	H45
Charge	0.17539	0.08505	0.23329	0.13921	0.12559
Atom	H46	O47	C48	C49	O50
Charge	0.21951	-0.22591	-0.14227	-0.01032	-0.29499
Atom	C51	C52	O53	C54	C55
Charge	-0.07269	0.01758	-0.38376	-0.00024	-0.03612
Atom	O56	C57	C58	O59	C60
Charge	-0.24037	-0.19412	-0.15911	-0.18991	-0.17586
Atom	C61	O62	C63	C64	O65
Charge	0.11129	-0.39586	0.08199	-0.14181	-0.26123
Atom	C66	C67	O68	C69	C70
Charge	-0.00679	-0.13467	-0.18180	-0.16442	0.10537
Atom	C71	S72	C73	S74	C75
Charge	-0.19027	0.16329	-0.10491	0.06950	-0.08224
Atom	S76	C77	C78	S79	C80
Charge	0.21154	-0.22148	0.03150	0.10142	-0.09899
Atom	H81	H82	H83	H84	H85
Charge	0.15476	0.15007	0.08359	0.13630	0.12166
Atom	H86	H87	H88	H89	H90
Charge	0.11182	0.11099	0.10584	0.10994	0.11166
Atom	H91	H92	H93	H94	H95
Charge	0.07276	0.12618	0.18688	0.21121	0.17761
Atom	H96	H97	H98	H99	H100
Charge	0.18128	0.14999	0.13384	0.04990	0.10624
Atom	H101	H102	H103	H104	H105
Charge	0.11881	0.00729	0.12578	0.15605	0.10111
Atom	H106	H107	H108	H109	H110
Charge	0.12828	0.13439	0.15507	0.17782	0.11600
Atom	H111	H112	H113	H114	C115
Charge	0.27708	0.30316	0.18681	0.16505	0.03135
Atom	C116	C117	C118	N119	C120
Charge	-0.09311	-0.12994	0.01078	-0.30564	0.35880
Atom	C121	C122	C123	C124	C125
Charge	-0.20124	0.08764	-0.26898	0.10219	0.17897
Atom	C126	C127	N128	C129	C130
Charge	-0.16640	-0.08591	-0.13350	0.28063	-0.16212
Atom	C131	C132	C133	C134	C135
Charge	0.02197	0.13375	-0.41043	0.15895	-0.21510
Atom	C136	C137	C138	C139	C140
Charge	-0.05287	-0.15731	-0.06099	-0.17739	-0.10599
Atom	C141	C142	C143	C144	H145
Charge	0.15789	-0.38439	0.09501	-0.12547	0.12980
Atom	H146	H147	H148	H149	H150
Charge	0.13093	0.25246	0.23614	0.23324	0.27475

DOI: 10.1038/NCHEM.749

Atom	H151	H152	H153	H154	H155
Charge	0.01069	0.09882	0.17910	0.05492	0.22262
Atom	H156	H157	H158	H159	H160
Charge	0.13048	0.14245	0.16365	0.14596	0.09633
Atom	H161	H162	H163	H164	O165
Charge	0.23081	0.13441	0.13349	0.22987	-0.25232
Atom	C166	C167	O168	C169	C170
Charge	-0.13373	-0.03938	-0.28864	-0.06331	0.01750
Atom	O171	C172	C173	O174	C175
Charge	-0.38156	-0.00651	-0.04345	-0.22526	-0.21784
Atom	C176	O177	C178	C179	O180
Charge	-0.15992	-0.19259	-0.19237	0.11738	-0.39533
Atom	C181	C182	O183	C184	C185
Charge	0.05502	-0.12772	-0.27010	-0.00544	-0.14003
Atom	O186	C187	C188	C189	S190
Charge	-0.17866	-0.16395	0.16180	-0.19901	0.23883
Atom	C191	S192	C193	S194	C195
Charge	0.03204	0.10452	-0.13876	0.34283	-0.22550
Atom	C196	S197	C198	H199	H200
Charge	0.06917	0.22424	-0.08301	0.15710	0.15635
Atom	H201	H202	H203	H204	H205
Charge	0.09808	0.14646	0.12035	0.11073	0.11303
Atom	H206	H207	H208	H209	H210
Charge	0.10280	0.11119	0.11500	0.08089	0.12797
Atom	H211	H212	H213	H214	H215
Charge	0.19040	0.21670	0.17950	0.18207	0.15479
Atom	H216	H217	H218	H219	H220
Charge	0.13937	0.04713	0.10626	0.12529	0.01719
Atom	H221	H222	H223	H224	H225
Charge	0.12401	0.15761	0.10173	0.13170	0.14474
Atom	H226	H227	H228	H229	H230
Charge	0.16042	0.18167	0.14848	0.30117	0.34284
Atom	H231	H232	C233	C234	C235
Charge	0.20567	0.18018	0.02541	-0.07512	-0.15004
Atom	C236				
Charge	0.03237				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.30003	0.38066	-0.19265	0.05808	-0.26656
Atom	C6	C7	C8	C9	N10
Charge	0.10154	0.24893	-0.20104	-0.06173	-0.18365
Atom	C11	C12	C13	C14	C15
Charge	0.35646	-0.23306	0.00773	0.15168	-0.39507
Atom	C16	C17	C18	C19	C20
Charge	0.12449	-0.17431	-0.09613	-0.12515	0.05548

Atom	C21	C22	C23	C24	C25
Charge	-0.26464	-0.05299	0.15517	-0.37833	0.05613
Atom	C26	H27	H28	H29	H30
Charge	-0.11211	0.11933	0.12104	0.25324	0.23362
Atom	H31	H32	H33	H34	H35
Charge	0.22787	0.27342	0.00272	0.12620	0.19018
Atom	H36	H37	H38	H39	H40
Charge	0.05391	0.22148	0.13904	0.14736	0.15211
Atom	H41	H42	H43	H44	H45
Charge	0.17434	0.07811	0.23896	0.15146	0.12804
Atom	H46	O47	C48	C49	O50
Charge	0.23125	-0.25309	-0.14900	-0.00995	-0.29413
Atom	C51	C52	O53	C54	C55
Charge	-0.07061	0.00995	-0.38225	0.00317	-0.05277
Atom	O56	C57	C58	O59	C60
Charge	-0.22333	-0.21972	-0.15823	-0.19391	-0.19324
Atom	C61	O62	C63	C64	O65
Charge	0.12226	-0.39596	0.06542	-0.12492	-0.27108
Atom	C66	C67	O68	C69	C70
Charge	-0.00648	-0.14182	-0.19078	-0.14710	0.12317
Atom	C71	S72	C73	S74	C75
Charge	-0.12988	0.24670	-0.11272	0.16363	-0.12585
Atom	S76	C77	C78	S79	C80
Charge	0.31165	-0.14253	0.02771	0.25916	-0.08835
Atom	H81	H82	H83	H84	H85
Charge	0.16861	0.16247	0.08359	0.14673	0.12656
Atom	H86	H87	H88	H89	H90
Charge	0.11210	0.11707	0.10919	0.11272	0.11529
Atom	H91	H92	H93	H94	H95
Charge	0.07236	0.13375	0.19304	0.22109	0.18014
Atom	H96	H97	H98	H99	H100
Charge	0.18445	0.15651	0.14053	0.04266	0.10933
Atom	H101	H102	H103	H104	H105
Charge	0.12395	0.01471	0.12401	0.15845	0.10548
Atom	H106	H107	H108	H109	H110
Charge	0.13548	0.14366	0.16798	0.20007	0.12353
Atom	H111	H112	H113	H114	C115
Charge	0.30307	0.32378	0.21336	0.18700	0.03582
Atom	C116	C117	C118	N119	C120
Charge	-0.09163	-0.13718	0.02461	-0.31528	0.35318
Atom	C121	C122	C123	C124	C125
Charge	-0.19339	0.08630	-0.27790	0.12067	0.18415
Atom	C126	C127	N128	C129	C130
Charge	-0.16948	-0.06322	-0.15650	0.29648	-0.16987
Atom	C131	C132	C133	C134	C135
Charge	0.02488	0.14068	-0.40016	0.17779	-0.27430
Atom	C136	C137	C138	C139	C140
Charge	-0.00715	-0.17336	-0.03293	-0.20260	-0.09625

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Atom	C141	C142	C143	C144	H145
Charge	0.17659	-0.38514	0.09561	-0.13375	0.13302
Atom	H146	H147	H148	H149	H150
Charge	0.13519	0.25538	0.23409	0.23266	0.27371
Atom	H151	H152	H153	H154	H155
Charge	0.00475	0.10285	0.18445	0.06355	0.22211
Atom	H156	H157	H158	H159	H160
Charge	0.13243	0.12649	0.16494	0.15183	0.09218
Atom	H161	H162	H163	H164	O165
Charge	0.23743	0.14045	0.13844	0.23709	-0.25808
Atom	C166	C167	O168	C169	C170
Charge	-0.14773	-0.02706	-0.28991	-0.06864	0.01791
Atom	O171	C172	C173	O174	C175
Charge	-0.38109	-0.00815	-0.04271	-0.22450	-0.22240
Atom	C176	O177	C178	C179	O180
Charge	-0.15943	-0.19553	-0.19708	0.12335	-0.39465
Atom	C181	C182	O183	C184	C185
Charge	0.04669	-0.11838	-0.27665	0.00039	-0.15926
Atom	O186	C187	C188	C189	S190
Charge	-0.16202	-0.15278	0.09450	-0.11034	0.19374
Atom	C191	S192	C193	S194	C195
Charge	0.05007	0.10468	-0.14541	0.32024	-0.14782
Atom	C196	S197	C198	H199	H200
Charge	0.00912	0.24007	-0.07393	0.16245	0.16078
Atom	H201	H202	H203	H204	H205
Charge	0.09619	0.14832	0.12320	0.11378	0.11569
Atom	H206	H207	H208	H209	H210
Charge	0.10245	0.11276	0.11701	0.07738	0.13072
Atom	H211	H212	H213	H214	H215
Charge	0.19155	0.21947	0.18064	0.18391	0.15668
Atom	H216	H217	H218	H219	H220
Charge	0.14165	0.04340	0.10688	0.12799	0.01997
Atom	H221	H222	H223	H224	H225
Charge	0.12165	0.15856	0.10216	0.13524	0.15154
Atom	H226	H227	H228	H229	H230
Charge	0.16748	0.18877	0.14586	0.29040	0.33819
Atom	H231	H232	C233	C234	C235
Charge	0.22107	0.18302	0.02734	-0.07593	-0.15046
Atom	C236				
Charge	0.03493				

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N1	5.8285999968	6.0184199672	5.4065661471
C2	4.5079513616	5.9166108206	5.6599111306
C3	3.5865236704	6.3209034412	4.7145438426
C4	3.9977519533	6.8415692176	3.4810252422
C5	5.3840963514	6.9834991408	3.2848480731
C6	6.2637139668	6.5606164434	4.2476595049

C7	3.0456726235	7.1489515169	2.4133265210
C8	1.6822935978	7.3701613595	2.6743287762
C9	0.7922338505	7.5309877751	1.6373526658
N10	1.2071700685	7.4863101197	0.3539288657
C11	2.5170898919	7.3366257132	0.0641278135
C12	3.4448560743	7.1768960713	1.0665575777
C13	0.2334943626	7.4261675304	-0.7713148416
C14	0.1135698807	6.0051578915	-1.2461261969
C15	-0.7180590341	5.1049668061	-0.5758106482
C16	-0.7500701528	3.7655102779	-0.9386891862
C17	0.0342855585	3.2853166748	-1.9969226295
C18	0.8401118143	4.2005483893	-2.6863522513
C19	0.8959205071	5.5362778695	-2.3055241535
C20	7.9985401398	1.7145872451	4.3755782185
C21	6.8784885393	1.7592869494	5.2180901109
C22	6.5215591060	2.9327636130	5.8696158296
C23	7.2860268870	4.0917315041	5.7140954273
C24	8.4273572080	4.0440962108	4.9106603008
C25	8.7750634863	2.8742342085	4.2460664775
C26	6.8179289168	5.3823327020	6.3196947215
H27	4.2305883621	5.4910588075	6.6252870520
H28	2.5339771959	6.1577280974	4.9360990708
H29	5.7835493160	7.4389606057	2.3828947851
H30	7.3415155699	6.6263207591	4.1300429774
H31	1.3058700880	7.4436093937	3.6910831717
H32	-0.2701884888	7.6984394085	1.7896262320
H33	2.7724410629	7.3152225010	-0.9924265945
H34	4.4756751042	7.0068619136	0.7647414039
H35	-0.7085311486	7.8269347886	-0.3851265240
H36	0.6153306019	8.1196910243	-1.5304971065
H37	-1.3515488810	5.4539226357	0.2414832537
H38	-1.4154610191	3.0822504983	-0.4133468083
H39	1.4678330770	3.8486061534	-3.5059374695
H40	1.5771949058	6.2221197454	-2.8111065376
H41	6.2538261552	0.8734093052	5.3286534439
H42	5.6225736101	2.9593432411	6.4881619066
H43	9.0655989526	4.9236392668	4.8168992246
H44	9.6818943499	2.8491059696	3.6431673741
H45	6.2987317784	5.2389258579	7.2718284862
H46	7.6247474942	6.1062812700	6.4747390580
O47	2.9617258729	3.2557424338	7.0029809794
C48	3.0852267814	3.0330037923	8.4091141427
C49	3.0377293967	4.3152306966	9.1989863666
O50	4.1566479853	5.1043825506	8.8362076086
C51	4.3059357748	6.2300600174	9.6945899566
C52	5.5427856642	6.9846684512	9.2767996195
O53	5.3951306070	7.5411068056	7.9749030303
C54	4.9490051100	8.8899660809	8.0125930793
C55	4.3638376041	9.2702770540	6.6783189457
O56	5.3363621344	9.0885511591	5.6536989462
C57	5.4377002398	10.1888552067	4.7617299108
C58	0.3703535112	11.5165593511	0.6057703553
O59	0.0854426166	10.5295999800	-0.3749678324
C60	-0.5990447934	11.1156785669	-1.4775113134
C61	-0.6833089994	10.1182623900	-2.5997365771
O62	0.6363198961	9.7703587240	-2.9660089357
C63	0.7009434403	8.8386585155	-4.0207732882
C64	2.1554677601	8.5927370461	-4.3260991939
O65	2.8078748128	8.1015535255	-3.1548263972
C66	4.2228537589	8.0683487642	-3.2642910207
C67	4.7637135749	6.6602659353	-3.2409286771
O68	4.5800961803	6.1197431207	-1.9328105352
C69	5.2003089414	4.8571051899	-1.8013801097
C70	4.9928738031	4.3522654370	-0.4115859100
C71	5.9525494864	4.1961864026	0.5200664182
S72	5.5253278362	3.5751181784	2.0978302057
C73	3.7880753882	3.6016851661	1.7435471981
S74	3.3581970669	3.9003348695	0.0657487715
C75	2.8462951683	3.4016506760	2.7104101981
S76	1.1116159160	3.5760241348	2.4299691570
C77	0.7358324435	3.5733971463	4.1460895633
C78	1.7189001331	3.3064478789	5.0238573042

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S79	3.3105569979	2.9831038603	4.3481130845
C80	1.6345511891	3.1979543634	6.5182193638
H81	4.0623276791	2.5566075817	8.5508239352
H82	2.3095479299	2.3341145302	8.7567075249
H83	2.0979645006	4.8694917907	9.0177922574
H84	3.0662367578	4.0750880859	10.2760008809
H85	4.3955918687	5.8951783277	10.7422514585
H86	3.4130187043	6.8777848162	9.6300769850
H87	5.7795028180	7.7648162175	10.0148380223
H88	6.4003103517	6.2996065660	9.2451896144
H89	5.7931072482	9.5538491238	8.2632202562
H90	4.1732403264	9.0258757054	8.7853740442
H91	3.4763972697	8.6529772936	6.4546559315
H92	4.0290573614	10.3170276044	6.7235334930
H93	6.3498321342	10.0103551176	4.1757834210
H94	5.6056621746	11.1259097294	5.3197158768
H95	-0.5433564266	11.7896555185	1.1646639392
H96	0.7160889411	12.4458295787	0.1170188891
H97	-0.0462355783	12.0045505962	-1.8232564754
H98	-1.6109339676	11.4437102072	-1.1865221704
H99	-1.2510092979	9.2185451397	-2.2943394840
H100	-1.2271536135	10.5682999185	-3.4467187205
H101	0.2015939165	9.2189110078	-4.9279786361
H102	0.1874867083	7.8971366225	-3.7408505646
H103	2.2487045780	7.8716039761	-5.1557592419
H104	2.6274759943	9.5366473395	-4.6371758545
H105	4.6453045707	8.6313494837	-2.4186167030
H106	4.5553495734	8.5649666839	-4.1861172012
H107	4.2521815705	6.0250663358	-3.9862662458
H108	5.8386417756	6.6708678606	-3.4884592838
H109	6.2832068351	4.9293040422	-2.0066006188
H110	4.7790076978	4.1464064927	-2.5391771373
H111	7.0027725476	4.4146371049	0.3387870139
H112	-0.3006242836	3.7464461984	4.4245017671
H113	1.0060568344	4.0072200816	6.9305763187
H114	1.1653144412	2.2432557659	6.8167228306
C115	1.4100308218	11.0735736196	1.5132836944
C116	2.3128967559	10.8130287718	2.2883725214
C117	3.3469070219	10.5524100245	3.1326387999
C118	4.2907919023	10.3540256782	3.8788280242
N119	1.5994025778	-2.8554989244	-2.7587851875
C120	1.6984524684	-3.6722354333	-1.6836489328
C121	2.9230537052	-3.9424210070	-1.1129898713
C122	4.1101873554	-3.3823806889	-1.6311318181
C123	3.9647793884	-2.6166222281	-2.8118468068
C124	2.7260183267	-2.3556645428	-3.3306912264
C125	5.3940333941	-3.4832080101	-0.9679285802
C126	5.5118350552	-3.8797405700	0.3837709346
C127	6.7088886761	-3.7827520527	1.0424360873
N128	7.8293665454	-3.3351646098	0.4129294636
C129	7.7827108625	-3.0424865121	-0.9093379959
C130	6.5997779899	-3.1138027983	-1.6045611258
C131	9.0455663873	-3.0441775658	1.2255569366
C132	8.8354489970	-1.8112959410	2.0634355023
C133	8.4102530439	-1.9174055854	3.3901714542
C134	8.1441694056	-0.7814443510	4.1455751384
C135	8.3147783742	0.4979073185	3.6028705656
C136	8.7673469905	0.5971487510	2.2785065004
C137	9.0124363331	-0.5377255378	1.5188991057
C138	0.0503554846	1.8506194490	-2.3356892983
C139	0.0341826188	0.8849008916	-1.3182839417
C140	0.0845679351	-0.4686915234	-1.6159619747
C141	0.1455702574	-0.8969020769	-2.9467189309
C142	0.1495661670	0.0563874494	-3.9653109460
C143	0.1049517600	1.4134923176	-3.6636841329
C144	0.2740402081	-2.3658903683	-3.2403489371
H145	0.7528277566	-4.0318584239	-1.2782132590
H146	2.9308881238	-4.5792437303	-0.2318269036
H147	4.8219368683	-2.1479511854	-3.2868138294
H148	2.5695632803	-1.7057549630	-4.1871627658
H149	4.6453482362	-4.2051285148	0.9539136198
H150	6.8198084895	-4.0145890966	2.0976298557

H151	8.7191058528	-2.7476290334	-1.3834994533
H152	6.6371365806	-2.8462911057	-2.6558469862
H153	9.2366159052	-3.9233369372	1.8507131400
H154	9.8747676943	-2.9370678729	0.5165421718
H155	8.3030970804	-2.9007264668	3.8500319291
H156	7.8367078728	-0.8883353531	5.1849080656
H157	9.3406766652	-0.4391319641	0.4848057872
H158	0.0129814330	1.2068253932	-0.2771940115
H159	0.0878460509	-1.2031285592	-0.8082060678
H160	0.1703465595	-0.2618517212	-5.0082195375
H161	0.0778985828	2.1426858964	-4.4722920401
H162	-0.4817975100	-2.9570848552	-2.7121743963
H163	0.2113203719	-2.5803279799	-4.3129746180
C164	1.1603603430	-2.6996345389	1.9382195368
O165	0.1752541389	-2.8353363434	0.9330568662
C166	-0.8699523827	-3.7168363790	1.3233466793
C167	-1.9054676537	-3.7083085211	0.2243645424
O168	-1.3707956762	-4.1317115005	-1.0236193869
C169	-1.7149531724	-5.4579222029	-1.4129511605
C170	-0.9454231084	-6.5187674316	-0.6459850689
O171	-1.1964186207	-7.7311237684	-1.3038127085
C172	-0.9080059426	-8.8913439629	-0.5488780650
C173	0.5571416123	-9.2455448530	-0.4985171268
O174	1.2499763180	-8.3229070172	0.3555861145
O175	8.8695995236	-3.8291322656	-4.1965680263
C176	10.1637973555	-4.4270939067	-4.1238171077
C177	10.7859269619	-4.0569757032	-2.7940710038
O178	10.7130562863	-2.6816619928	-2.4715519895
C179	11.3651209490	-1.8402731145	-3.4247771719
C180	11.4082978469	-0.4188181106	-2.9082202241
O181	10.1948852660	0.3073615602	-3.0323727855
C182	9.1334291139	-0.2960971807	-2.3496599981
C183	8.0981823216	0.7446460308	-1.9921472152
O184	7.0182469446	0.0334722709	-1.4022809893
C185	6.1366281053	0.8948395413	-0.7141384377
H186	1.5351860954	-3.6956100507	2.2497800670
H187	0.7319146122	-2.2414727218	2.8491816015
H188	-1.3271520975	-3.3806775883	2.2702528152
H189	-0.4599091549	-4.7293349299	1.4915246109
H190	-2.7629991984	-4.3331153300	0.5143162133
H191	-2.2715863463	-2.6832145487	0.0819787719
H192	-1.4624311560	-5.5357341537	-2.4777465925
H193	-2.7988264487	-5.6195418305	-1.3195708302
H194	0.1343045915	-6.2635090123	-0.6255581185
H195	-1.2738271619	-6.5729288025	0.4101899538
H196	-1.4411748109	-9.7074319299	-1.0483340645
H197	-1.3049944694	-8.7970554155	0.4758311024
H198	0.6647332786	-10.2675015039	-0.1029946668
H199	0.9880121625	-9.2265384364	-1.5132260534
H200	10.7781507310	-4.0863075824	-4.9720826218
H201	10.0995294389	-5.5255063890	-4.1903814011
H202	10.2571991212	-4.5728349029	-1.9798732906
H203	11.8321623639	-4.4074414111	-2.7866104271
H204	10.8360510417	-1.8693431463	-4.3909580673
H205	12.3951151625	-2.1990620433	-3.5875645221
H206	11.7315525648	-0.4319101365	-1.8518369241
H207	12.1436270267	0.1526251257	-3.4822099618
H208	9.4977958442	-0.7711026725	-1.4220573104
H209	8.6663160848	-1.1007543430	-2.9478570696
H210	8.5191841259	1.4733898506	-1.2750183990
H211	7.7652726917	1.3075888156	-2.8807063338
H212	5.6995845736	1.6451336894	-1.4031306529
C213	8.0528453878	-4.3394078953	-5.2373362837
H214	7.7227271040	-3.5137045571	-5.8825412766
H215	8.6147090244	-5.0447946701	-5.8683553592
C216	2.5005699673	-8.7840631368	0.8041368667
H217	2.6085627822	-9.8655822467	0.6232487402
C218	5.5969775864	-5.0597539424	-5.1247602990
C219	6.8488381283	-5.0077626921	-4.6349099659
S220	7.1035203611	-5.7824078682	-3.0815597849
C221	5.4255664556	-6.2018937717	-2.8380034920
S222	4.3671970344	-5.8692334284	-4.1974155514

DOI: 10.1038/NCHEM.749

C223	4.9941329684	-6.8007779081	-1.6717701562
S224	6.0961973559	-7.1683608293	-0.3602962310
C225	4.8971410250	-7.9501065661	0.6197705622
C226	3.6428514288	-8.0587863310	0.1420271554
S227	3.3411516645	-7.3237004798	-1.4225139254
H228	5.2987431002	-4.6406378379	-6.0819300137
H229	2.5625622660	-8.6341675825	1.8913921850
H230	5.2259022154	-8.3701400005	1.5665446064
H231	6.6849907210	1.4704043479	0.0580098490
C232	2.2516530429	-1.8946899757	1.4264176421
C233	3.1593582645	-1.2302793779	0.9615389842
C234	4.1715225172	-0.5066585028	0.4135669092
C235	5.0777697074	0.1273820410	-0.0930191092
H236	8.9032237915	1.5833776348	1.8325726767

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.14408	0.24141	-0.12329	0.08481	-0.24768
Atom	C6	C7	C8	C9	N10
Charge	-0.00815	0.13826	-0.15626	-0.16233	-0.07088
Atom	C11	C12	C13	C14	C15
Charge	0.28768	-0.15600	-0.04026	0.08942	-0.33490
Atom	C16	C17	C18	C19	C20
Charge	-0.06252	0.02989	-0.15730	-0.13446	-0.27087
Atom	C21	C22	C23	C24	C25
Charge	0.06749	-0.28413	0.20448	-0.42659	0.12823
Atom	C26	H27	H28	H29	H30
Charge	-0.13847	0.14541	0.13269	0.23928	0.23410
Atom	H31	H32	H33	H34	H35
Charge	0.22116	0.27000	-0.02081	0.11639	0.15672
Atom	H36	H37	H38	H39	H40
Charge	0.05942	0.21617	0.15820	0.16221	0.18415
Atom	H41	H42	H43	H44	H45
Charge	0.11272	0.14811	0.22456	0.10627	0.11911
Atom	H46	O47	C48	C49	O50
Charge	0.18771	-0.19137	-0.06282	-0.07631	-0.26048
Atom	C51	C52	O53	C54	C55
Charge	-0.07605	0.02091	-0.36031	-0.02015	0.02466
Atom	O56	C57	C58	O59	C60
Charge	-0.28278	-0.16713	-0.11589	-0.19608	-0.17474
Atom	C61	O62	C63	C64	O65
Charge	0.08620	-0.38568	0.08625	-0.15730	-0.26383
Atom	C66	C67	O68	C69	C70
Charge	0.06484	-0.13885	-0.16098	-0.20313	0.05136
Atom	C71	S72	C73	S74	C75
Charge	-0.29339	0.11468	-0.05611	0.00247	-0.01450
Atom	S76	C77	C78	S79	C80
Charge	0.09886	-0.36968	0.07985	-0.11234	-0.11201
Atom	H81	H82	H83	H84	H85
Charge	0.11329	0.12040	0.10371	0.12521	0.11416

Atom	H86	H87	H88	H89	H90
Charge	0.10770	0.09907	0.09772	0.10141	0.10593
Atom	H91	H92	H93	H94	H95
Charge	0.07003	0.10531	0.18606	0.19582	0.15788
Atom	H96	H97	H98	H99	H100
Charge	0.15886	0.14885	0.12936	0.06876	0.10029
Atom	H101	H102	H103	H104	H105
Charge	0.11194	0.00683	0.13231	0.14415	0.07476
Atom	H106	H107	H108	H109	H110
Charge	0.09759	0.11346	0.13151	0.13817	0.17173
Atom	H111	H112	H113	H114	C115
Charge	0.24499	0.29025	0.14081	0.14881	0.03807
Atom	C116	C117	C118	N119	C120
Charge	-0.12090	-0.10533	-0.00929	0.02550	-0.00491
Atom	C121	C122	C123	C124	C125
Charge	-0.37651	0.53476	-0.50250	0.12656	0.56747
Atom	C126	C127	N128	C129	C130
Charge	-0.34063	-0.01441	-0.00248	0.54672	-0.76026
Atom	C131	C132	C133	C134	C135
Charge	-0.37432	0.22880	-0.34827	-0.05758	0.05691
Atom	C136	C137	C138	C139	C140
Charge	-0.16928	-0.19181	-0.13051	0.02790	-0.23853
Atom	C141	C142	C143	C144	H145
Charge	0.10969	-0.27500	-0.06808	-0.19069	0.20695
Atom	H146	H147	H148	H149	H150
Charge	0.20839	0.24377	0.20461	0.17207	0.23072
Atom	H151	H152	H153	H154	H155
Charge	-0.15813	0.30551	0.23103	0.21259	0.21298
Atom	H156	H157	H158	H159	H160
Charge	0.16406	0.11459	0.05953	0.16647	0.19794
Atom	H161	H162	H163	C164	O165
Charge	0.15210	0.13310	0.19228	-0.00516	-0.22630
Atom	C166	C167	O168	C169	C170
Charge	-0.06459	-0.03495	-0.27289	-0.22379	0.29600
Atom	O171	C172	C173	O174	O175
Charge	-0.47750	0.01566	0.15491	-0.40618	-0.18032
Atom	C176	C177	O178	C179	C180
Charge	0.01399	-0.15390	-0.28740	-0.09474	0.06991
Atom	O181	C182	C183	O184	C185
Charge	-0.55425	0.52690	-0.22993	-0.44651	0.73901
Atom	H186	H187	H188	H189	H190
Charge	0.12072	0.14296	0.13068	0.05571	0.13895
Atom	H191	H192	H193	H194	H195
Charge	0.09344	0.13734	0.14598	0.01533	0.06075
Atom	H196	H197	H198	H199	H200
Charge	0.11687	0.07570	0.07124	0.04086	0.09273
Atom	H201	H202	H203	H204	H205
Charge	0.10876	0.13373	0.14924	0.12802	0.12954

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Atom	H206	H207	H208	H209	H210
Charge	0.05711	0.13001	0.04711	-0.02566	0.09064
Atom	H211	H212	C213	H214	H215
Charge	0.12683	-0.03414	-0.18570	0.15453	0.17804
Atom	C216	H217	C218	C219	S220
Charge	0.04790	0.11793	-0.21167	0.01973	-0.06451
Atom	C221	S222	C223	S224	C225
Charge	-0.10397	0.00156	-0.06439	0.01184	-0.24427
Atom	C226	S227	H228	H229	H230
Charge	-0.03118	0.00200	0.27414	0.11835	0.27041
Atom	H231	C232	C233	C234	C235
Charge	-0.06359	-0.05936	-0.14616	0.12755	-0.47619
Atom	H236				
Charge	0.19458				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.22689	0.13337	-0.03069	0.06494	-0.27878
Atom	C6	C7	C8	C9	N10
Charge	0.07659	0.12601	-0.23064	-0.10751	-0.14575
Atom	C11	C12	C13	C14	C15
Charge	0.36214	-0.13757	-0.05509	0.06524	-0.30185
Atom	C16	C17	C18	C19	C20
Charge	-0.08750	0.00623	-0.13266	-0.11456	-0.17038
Atom	C21	C22	C23	C24	C25
Charge	-0.02095	-0.22001	0.16745	-0.40512	0.10488
Atom	C26	H27	H28	H29	H30
Charge	-0.10061	0.18940	0.09983	0.25144	0.22508
Atom	H31	H32	H33	H34	H35
Charge	0.25399	0.27379	-0.07263	0.10444	0.17704
Atom	H36	H37	H38	H39	H40
Charge	0.10835	0.20557	0.17161	0.15205	0.17153
Atom	H41	H42	H43	H44	H45
Charge	0.12207	0.13256	0.23004	0.11415	0.11791
Atom	H46	O47	C48	C49	O50
Charge	0.20058	-0.24015	-0.05797	-0.09353	-0.26150
Atom	C51	C52	O53	C54	C55
Charge	-0.06264	-0.00341	-0.34744	-0.02179	0.00307
Atom	O56	C57	C58	O59	C60
Charge	-0.25108	-0.21780	-0.12155	-0.19136	-0.21279
Atom	C61	O62	C63	C64	O65
Charge	0.10270	-0.39515	0.08169	-0.15305	-0.25458
Atom	C66	C67	O68	C69	C70
Charge	0.03262	-0.12523	-0.15332	-0.31403	0.17354
Atom	C71	S72	C73	S74	C75

Charge	-0.30362	0.20369	-0.04686	0.09878	-0.05451
Atom	S76	C77	C78	S79	C80
Charge	0.27083	-0.31192	0.05751	0.13032	-0.07585
Atom	H81	H82	H83	H84	H85
Charge	0.12422	0.13145	0.11060	0.13785	0.11789
Atom	H86	H87	H88	H89	H90
Charge	0.10585	0.10871	0.10314	0.10496	0.11116
Atom	H91	H92	H93	H94	H95
Charge	0.07837	0.11235	0.19521	0.21138	0.16241
Atom	H96	H97	H98	H99	H100
Charge	0.16144	0.16295	0.14072	0.05943	0.10420
Atom	H101	H102	H103	H104	H105
Charge	0.11589	0.00753	0.13282	0.15002	0.08561
Atom	H106	H107	H108	H109	H110
Charge	0.10991	0.12484	0.14309	0.18036	0.20604
Atom	H111	H112	H113	H114	C115
Charge	0.28330	0.31374	0.16087	0.16214	0.04362
Atom	C116	C117	C118	N119	C120
Charge	-0.11094	-0.12022	0.01828	0.02253	0.01212
Atom	C121	C122	C123	C124	C125
Charge	-0.37971	0.52839	-0.47804	0.10040	0.48733
Atom	C126	C127	N128	C129	C130
Charge	-0.29177	-0.05548	0.01507	0.51453	-0.68788
Atom	C131	C132	C133	C134	C135
Charge	-0.38342	0.25609	-0.34227	-0.06284	-0.00288
Atom	C136	C137	C138	C139	C140
Charge	-0.12265	-0.22878	-0.05021	-0.08963	-0.15987
Atom	C141	C142	C143	C144	H145
Charge	0.07891	-0.24790	-0.10683	-0.16902	0.19799
Atom	H146	H147	H148	H149	H150
Charge	0.20890	0.24358	0.20887	0.16604	0.23747
Atom	H151	H152	H153	H154	H155
Charge	-0.14729	0.28879	0.23855	0.21746	0.21406
Atom	H156	H157	H158	H159	H160
Charge	0.17588	0.13238	0.10051	0.13678	0.20100
Atom	H161	H162	H163	C164	O165
Charge	0.16689	0.13017	0.19573	-0.03013	-0.21861
Atom	C166	C167	O168	C169	C170
Charge	-0.06080	-0.04596	-0.26654	-0.22835	0.29931
Atom	O171	C172	C173	O174	O175
Charge	-0.47418	0.00855	0.16189	-0.40914	-0.18186
Atom	C176	C177	O178	C179	C180
Charge	0.01677	-0.16323	-0.28694	-0.09190	0.06455
Atom	O181	C182	C183	O184	C185
Charge	-0.55139	0.53599	-0.23407	-0.41022	0.56991
Atom	H186	H187	H188	H189	H190
Charge	0.13090	0.14805	0.12999	0.06028	0.14345
Atom	H191	H192	H193	H194	H195

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Charge	0.09627	0.13802	0.14818	0.01273	0.05992
Atom	H196	H197	H198	H199	H200
Charge	0.11868	0.07729	0.07059	0.04048	0.09353
Atom	H201	H202	H203	H204	H205
Charge	0.11030	0.13500	0.15289	0.12866	0.13155
Atom	H206	H207	H208	H209	H210
Charge	0.05944	0.13200	0.03354	-0.02701	0.09015
Atom	H211	H212	C213	H214	H215
Charge	0.13179	0.00683	-0.18695	0.15433	0.17988
Atom	C216	H217	C218	C219	S220
Charge	0.04792	0.12007	-0.21058	0.02083	-0.06269
Atom	C221	S222	C223	S224	C225
Charge	-0.10301	0.00651	-0.06133	0.01866	-0.24813
Atom	C226	S227	H228	H229	H230
Charge	-0.02879	0.00360	0.27474	0.11768	0.27130
Atom	H231	C232	C233	C234	C235
Charge	-0.03069	-0.03144	-0.15485	0.08798	-0.39475
Atom	H236				
Charge	0.17872				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.17465	0.29077	-0.14331	0.11773	-0.29962
Atom	C6	C7	C8	C9	N10
Charge	0.03019	0.12234	-0.14127	-0.17743	-0.04588
Atom	C11	C12	C13	C14	C15
Charge	0.24413	-0.11576	-0.04463	0.09521	-0.33740
Atom	C16	C17	C18	C19	C20
Charge	-0.07560	0.05400	-0.19421	-0.11112	-0.25042
Atom	C21	C22	C23	C24	C25
Charge	0.05143	-0.27173	0.20441	-0.43376	0.12927
Atom	C26	H27	H28	H29	H30
Charge	-0.12459	0.12726	0.13599	0.25025	0.22844
Atom	H31	H32	H33	H34	H35
Charge	0.21907	0.27323	0.00127	0.09784	0.15927
Atom	H36	H37	H38	H39	H40
Charge	0.05292	0.21745	0.16852	0.16918	0.18397
Atom	H41	H42	H43	H44	H45
Charge	0.11150	0.14996	0.22866	0.11067	0.11254
Atom	H46	O47	C48	C49	O50
Charge	0.18776	-0.19029	-0.06254	-0.07738	-0.25785
Atom	C51	C52	O53	C54	C55
Charge	-0.07911	0.01749	-0.35847	-0.02445	0.03054
Atom	O56	C57	C58	O59	C60
Charge	-0.28864	-0.16601	-0.11839	-0.19807	-0.17130

Atom	C61	O62	C63	C64	O65
Charge	0.08075	-0.38241	0.08771	-0.16111	-0.26844
Atom	C66	C67	O68	C69	C70
Charge	0.06458	-0.12217	-0.18057	-0.20084	0.07638
Atom	C71	S72	C73	S74	C75
Charge	-0.24381	0.10208	-0.08756	-0.00668	-0.02573
Atom	S76	C77	C78	S79	C80
Charge	0.11081	-0.37942	0.09029	-0.11521	-0.11870
Atom	H81	H82	H83	H84	H85
Charge	0.11191	0.12071	0.10488	0.12581	0.11500
Atom	H86	H87	H88	H89	H90
Charge	0.11001	0.10087	0.09895	0.10252	0.10757
Atom	H91	H92	H93	H94	H95
Charge	0.06637	0.10623	0.18675	0.19616	0.15887
Atom	H96	H97	H98	H99	H100
Charge	0.16020	0.14860	0.12920	0.07120	0.10148
Atom	H101	H102	H103	H104	H105
Charge	0.11285	0.00407	0.13264	0.14651	0.07630
Atom	H106	H107	H108	H109	H110
Charge	0.09778	0.11008	0.12699	0.14045	0.16635
Atom	H111	H112	H113	H114	C115
Charge	0.22648	0.29406	0.14474	0.14987	0.04141
Atom	C116	C117	C118	N119	C120
Charge	-0.12356	-0.10670	-0.00760	0.10929	-0.15431
Atom	C121	C122	C123	C124	C125
Charge	-0.37540	0.44088	-0.49977	0.11101	0.73426
Atom	C126	C127	N128	C129	C130
Charge	-0.47720	0.05522	-0.03992	0.60736	-1.06171
Atom	C131	C132	C133	C134	C135
Charge	-0.34152	0.23671	-0.34097	-0.06451	0.04113
Atom	C136	C137	C138	C139	C140
Charge	-0.14373	-0.20782	-0.10601	-0.02553	-0.22013
Atom	C141	C142	C143	C144	H145
Charge	0.16946	-0.29486	-0.07702	-0.26122	0.32581
Atom	H146	H147	H148	H149	H150
Charge	0.13899	0.27528	0.22101	0.20265	0.23888
Atom	H151	H152	H153	H154	H155
Charge	-0.16566	0.28253	0.22527	0.22222	0.21194
Atom	H156	H157	H158	H159	H160
Charge	0.17356	0.10743	0.06772	0.15704	0.20779
Atom	H161	H162	H163	C164	O165
Charge	0.16064	0.15171	0.20700	-0.07277	-0.16134
Atom	C166	C167	O168	C169	C170
Charge	-0.14059	-0.00289	-0.32936	-0.13977	0.17127
Atom	O171	C172	C173	O174	O175
Charge	-0.45564	0.00589	0.06836	-0.42209	-0.19512
Atom	C176	C177	O178	C179	C180
Charge	-0.20078	-0.03928	-0.31368	-0.09045	0.02486

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Atom	O181	C182	C183	O184	C185
Charge	-0.50614	0.44059	-0.42000	-0.16870	0.31029
Atom	H186	H187	H188	H189	H190
Charge	0.14909	0.15353	0.15557	0.06620	0.14077
Atom	H191	H192	H193	H194	H195
Charge	0.09328	0.12150	0.14874	0.01065	0.10494
Atom	H196	H197	H198	H199	H200
Charge	0.13254	0.10136	0.09802	0.09224	0.15482
Atom	H201	H202	H203	H204	H205
Charge	0.17870	0.09032	0.15508	0.13291	0.13813
Atom	H206	H207	H208	H209	H210
Charge	0.07355	0.14398	0.08541	0.02290	0.16623
Atom	H211	H212	C213	H214	H215
Charge	0.17107	0.03963	-0.02749	0.15141	0.17705
Atom	C216	H217	C218	C219	S220
Charge	0.16470	0.14063	-0.17340	0.00834	0.34107
Atom	C221	S222	C223	S224	C225
Charge	-0.07719	0.42573	-0.00880	0.41386	-0.20858
Atom	C226	S227	H228	H229	H230
Charge	-0.05586	0.32378	0.30923	0.11651	0.31928
Atom	H231	C232	C233	C234	C235
Charge	-0.00410	-0.04534	-0.09670	0.05215	-0.25940
Atom	H236				
Charge	0.18841				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.25740	0.18205	-0.05176	0.09860	-0.33180
Atom	C6	C7	C8	C9	N10
Charge	0.11506	0.10953	-0.21482	-0.12279	-0.12201
Atom	C11	C12	C13	C14	C15
Charge	0.31917	-0.09710	-0.05792	0.06992	-0.30313
Atom	C16	C17	C18	C19	C20
Charge	-0.10030	0.02994	-0.16900	-0.09064	-0.15027
Atom	C21	C22	C23	C24	C25
Charge	-0.03704	-0.20758	0.16670	-0.41208	0.10621
Atom	C26	H27	H28	H29	H30
Charge	-0.08623	0.17187	0.10349	0.26270	0.21953
Atom	H31	H32	H33	H34	H35
Charge	0.25128	0.27662	-0.05101	0.08572	0.17944
Atom	H36	H37	H38	H39	H40
Charge	0.10173	0.20626	0.18128	0.15883	0.17107
Atom	H41	H42	H43	H44	H45
Charge	0.12099	0.13421	0.23405	0.11860	0.11119

Atom	H46	O47	C48	C49	O50
Charge	0.20054	-0.23947	-0.05737	-0.09478	-0.25909
Atom	C51	C52	O53	C54	C55
Charge	-0.06551	-0.00683	-0.34578	-0.02580	0.00874
Atom	O56	C57	C58	O59	C60
Charge	-0.25660	-0.21700	-0.12401	-0.19289	-0.21040
Atom	C61	O62	C63	C64	O65
Charge	0.09796	-0.39267	0.08200	-0.15729	-0.25881
Atom	C66	C67	O68	C69	C70
Charge	0.03193	-0.10814	-0.17287	-0.31253	0.19855
Atom	C71	S72	C73	S74	C75
Charge	-0.25430	0.19143	-0.07823	0.08955	-0.06599
Atom	S76	C77	C78	S79	C80
Charge	0.28231	-0.32163	0.06842	0.12870	-0.08283
Atom	H81	H82	H83	H84	H85
Charge	0.12296	0.13192	0.11158	0.13866	0.11888
Atom	H86	H87	H88	H89	H90
Charge	0.10801	0.11074	0.10436	0.10628	0.11265
Atom	H91	H92	H93	H94	H95
Charge	0.07453	0.11334	0.19574	0.21191	0.16318
Atom	H96	H97	H98	H99	H100
Charge	0.16273	0.16262	0.14071	0.06217	0.10572
Atom	H101	H102	H103	H104	H105
Charge	0.11704	0.00718	0.13311	0.15228	0.08694
Atom	H106	H107	H108	H109	H110
Charge	0.11032	0.12146	0.13853	0.18264	0.20084
Atom	H111	H112	H113	H114	C115
Charge	0.26477	0.31724	0.16493	0.16341	0.04674
Atom	C116	C117	C118	N119	C120
Charge	-0.11359	-0.12168	0.02006	0.10608	-0.13644
Atom	C121	C122	C123	C124	C125
Charge	-0.37754	0.43441	-0.47450	0.08606	0.64984
Atom	C126	C127	N128	C129	C130
Charge	-0.42766	0.01651	-0.02195	0.57404	-0.98357
Atom	C131	C132	C133	C134	C135
Charge	-0.34989	0.26287	-0.33505	-0.06950	-0.01838
Atom	C136	C137	C138	C139	C140
Charge	-0.09751	-0.24487	-0.02513	-0.14349	-0.14160
Atom	C141	C142	C143	C144	H145
Charge	0.13793	-0.26756	-0.11602	-0.23880	0.31745
Atom	H146	H147	H148	H149	H150
Charge	0.13988	0.27481	0.22479	0.19713	0.24568
Atom	H151	H152	H153	H154	H155
Charge	-0.15415	0.26561	0.23294	0.22691	0.21317
Atom	H156	H157	H158	H159	H160
Charge	0.18538	0.12521	0.10876	0.12706	0.21079
Atom	H161	H162	H163	C164	O165
Charge	0.17581	0.14865	0.21052	-0.09757	-0.15452

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Atom	C166	C167	O168	C169	C170
Charge	-0.13654	-0.01386	-0.32328	-0.14480	0.17538
Atom	O171	C172	C173	O174	O175
Charge	-0.45264	-0.00213	0.07690	-0.42580	-0.19704
Atom	C176	C177	O178	C179	C180
Charge	-0.19618	-0.04956	-0.31324	-0.08736	0.01953
Atom	O181	C182	C183	O184	C185
Charge	-0.50359	0.45029	-0.42225	-0.13494	0.14366
Atom	H186	H187	H188	H189	H190
Charge	0.15968	0.15845	0.15468	0.07135	0.14550
Atom	H191	H192	H193	H194	H195
Charge	0.09569	0.12209	0.15102	0.00706	0.10406
Atom	H196	H197	H198	H199	H200
Charge	0.13499	0.10268	0.09996	0.09089	0.15501
Atom	H201	H202	H203	H204	H205
Charge	0.17988	0.09214	0.15890	0.13331	0.14029
Atom	H206	H207	H208	H209	H210
Charge	0.07584	0.14592	0.07133	0.02133	0.16492
Atom	H211	H212	C213	H214	H215
Charge	0.17561	0.08024	-0.02868	0.15065	0.17875
Atom	C216	H217	C218	C219	S220
Charge	0.16321	0.14552	-0.17164	0.00886	0.34099
Atom	C221	S222	C223	S224	C225
Charge	-0.07738	0.42821	-0.00833	0.41947	-0.21182
Atom	C226	S227	H228	H229	H230
Charge	-0.05170	0.32568	0.30884	0.11571	0.31997
Atom	H231	C232	C233	C234	C235
Charge	0.02895	-0.01713	-0.10609	0.01272	-0.17903
Atom	H236				
Charge	0.17290				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	-0.33129	0.07168	0.03266	0.08459	-0.35840
Atom	C6	C7	C8	C9	N10
Charge	0.18568	0.09064	-0.28306	-0.07267	-0.19693
Atom	C11	C12	C13	C14	C15
Charge	0.39729	-0.08433	-0.06557	0.04085	-0.27198
Atom	C16	C17	C18	C19	C20
Charge	-0.11685	0.01499	-0.15314	-0.06374	-0.05886
Atom	C21	C22	C23	C24	C25
Charge	-0.10988	-0.15368	0.13908	-0.39415	0.08523
Atom	C26	H27	H28	H29	H30
Charge	-0.05467	0.21749	0.07385	0.27331	0.21316
Atom	H31	H32	H33	H34	H35

Charge	0.28140	0.27996	-0.10514	0.07723	0.19794
Atom	H36	H37	H38	H39	H40
Charge	0.14649	0.19642	0.19069	0.15137	0.15718
Atom	H41	H42	H43	H44	H45
Charge	0.12735	0.12101	0.23959	0.12736	0.11076
Atom	H46	O47	C48	C49	O50
Charge	0.21359	-0.28636	-0.04700	-0.11013	-0.26126
Atom	C51	C52	O53	C54	C55
Charge	-0.05232	-0.02929	-0.33363	-0.02709	-0.01383
Atom	O56	C57	C58	O59	C60
Charge	-0.22277	-0.26855	-0.12775	-0.18788	-0.24732
Atom	C61	O62	C63	C64	O65
Charge	0.11563	-0.40276	0.07865	-0.15317	-0.24930
Atom	C66	C67	O68	C69	C70
Charge	0.00393	-0.09574	-0.16896	-0.40307	0.30669
Atom	C71	S72	C73	S74	C75
Charge	-0.24910	0.27579	-0.05983	0.18039	-0.10879
Atom	S76	C77	C78	S79	C80
Charge	0.43305	-0.24280	0.06739	0.34916	-0.06380
Atom	H81	H82	H83	H84	H85
Charge	0.13302	0.14230	0.11830	0.15024	0.12259
Atom	H86	H87	H88	H89	H90
Charge	0.10604	0.11973	0.10944	0.10967	0.11766
Atom	H91	H92	H93	H94	H95
Charge	0.08291	0.12011	0.20531	0.22706	0.16675
Atom	H96	H97	H98	H99	H100
Charge	0.16454	0.17612	0.15142	0.05099	0.10948
Atom	H101	H102	H103	H104	H105
Charge	0.12025	0.01040	0.13383	0.15715	0.09646
Atom	H106	H107	H108	H109	H110
Charge	0.12185	0.13367	0.14915	0.22122	0.23241
Atom	H111	H112	H113	H114	C115
Charge	0.30132	0.33867	0.19005	0.18503	0.05065
Atom	C116	C117	C118	N119	C120
Charge	-0.10231	-0.13759	0.04848	0.10743	-0.12320
Atom	C121	C122	C123	C124	C125
Charge	-0.37669	0.42366	-0.44504	0.05767	0.57619
Atom	C126	C127	N128	C129	C130
Charge	-0.38104	-0.01953	-0.00651	0.54241	-0.91296
Atom	C131	C132	C133	C134	C135
Charge	-0.35526	0.28516	-0.32873	-0.07267	-0.07457
Atom	C136	C137	C138	C139	C140
Charge	-0.05515	-0.27636	0.03808	-0.24140	-0.07804
Atom	C141	C142	C143	C144	H145
Charge	0.11730	-0.24607	-0.14676	-0.22224	0.31122
Atom	H146	H147	H148	H149	H150
Charge	0.13950	0.27314	0.22939	0.19159	0.25209
Atom	H151	H152	H153	H154	H155

DOI: 10.1038/NCHEM.749

Charge	-0.14260	0.24989	0.23995	0.23040	0.21455
Atom	H156	H157	H158	H159	H160
Charge	0.19589	0.14207	0.14303	0.10129	0.21404
Atom	H161	H162	H163	C164	O165
Charge	0.18980	0.14648	0.21463	-0.12127	-0.14871
Atom	C166	C167	O168	C169	C170
Charge	-0.13215	-0.02455	-0.31725	-0.14970	0.17997
Atom	O171	C172	C173	O174	O175
Charge	-0.45062	-0.00793	0.08845	-0.43085	-0.20004
Atom	C176	C177	O178	C179	C180
Charge	-0.19037	-0.05856	-0.31289	-0.08398	0.01558
Atom	O181	C182	C183	O184	C185
Charge	-0.50141	0.46023	-0.42750	-0.10244	-0.00361
Atom	H186	H187	H188	H189	H190
Charge	0.17031	0.16306	0.15375	0.07612	0.14966
Atom	H191	H192	H193	H194	H195
Charge	0.09822	0.12270	0.15300	0.00317	0.10316
Atom	H196	H197	H198	H199	H200
Charge	0.13665	0.10334	0.09909	0.08945	0.15449
Atom	H201	H202	H203	H204	H205
Charge	0.18072	0.09367	0.16193	0.13354	0.14192
Atom	H206	H207	H208	H209	H210
Charge	0.07758	0.14727	0.05710	0.02039	0.16496
Atom	H211	H212	C213	H214	H215
Charge	0.18040	0.11665	-0.02881	0.14978	0.17990
Atom	C216	H217	C218	C219	S220
Charge	0.16483	0.14898	-0.17066	0.00934	0.34023
Atom	C221	S222	C223	S224	C225
Charge	-0.07703	0.43148	-0.00444	0.42293	-0.21414
Atom	C226	S227	H228	H229	H230
Charge	-0.04970	0.32713	0.30862	0.11471	0.32079
Atom	H231	C232	C233	C234	C235
Charge	0.05617	0.01002	-0.11565	-0.02123	-0.11137
Atom	H236				
Charge	0.15634				

Out – Out

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	0.11364	-0.00944	-0.33946	0.45731	-0.47134
Atom	C6	C7	C8	C9	N10
Charge	0.05664	0.42412	-0.06794	-0.23899	0.19589
Atom	C11	C12	C13	C14	C15
Charge	0.13468	-0.34086	-0.41744	0.22431	-0.30876
Atom	C16	C17	C18	C19	C20

Charge	-0.05073	-0.03213	-0.09157	-0.26228	0.03089
Atom	C21	C22	C23	C24	C25
Charge	-0.17859	-0.15418	0.15043	-0.25724	-0.17190
Atom	C26	H27	H28	H29	H30
Charge	-0.29524	0.22719	0.16719	0.28628	0.21278
Atom	H31	H32	H33	H34	H35
Charge	0.10625	0.26859	0.01246	0.09184	0.23405
Atom	H36	H37	H38	H39	H40
Charge	0.23457	0.20691	0.13083	0.18793	0.17715
Atom	H41	H42	H43	H44	H45
Charge	0.12576	0.20301	0.17272	0.16185	0.20469
Atom	C46	O47	C48	C49	O50
Charge	0.00114	-0.27029	-0.05050	-0.02799	-0.28467
Atom	C51	C52	O53	C54	C55
Charge	-0.24817	0.27135	-0.46034	-0.03787	-0.00305
Atom	O56	O57	C58	C59	O60
Charge	-0.36678	-0.07416	-0.04528	-0.18713	-0.28271
Atom	C61	C62	O63	C64	C65
Charge	-0.10556	0.12459	-0.52469	0.18897	0.14514
Atom	O66	C67	H68	H69	H70
Charge	-0.67760	0.88296	0.13729	0.15776	0.13447
Atom	H71	H72	H73	H74	H75
Charge	0.04749	0.13346	0.09530	0.13929	0.15760
Atom	H76	H77	H78	H79	H80
Charge	0.02803	0.09052	0.14287	0.09937	0.12616
Atom	H81	H82	H83	H84	H85
Charge	0.07591	0.10003	0.11656	0.14557	0.16006
Atom	H86	H87	H88	H89	H90
Charge	0.12716	0.12858	0.04295	0.10736	0.15807
Atom	H91	H92	H93	H94	C95
Charge	0.07250	-0.01034	0.04004	-0.05199	-0.19841
Atom	H96	H97	C98	H99	C100
Charge	0.12829	0.16830	0.07863	0.10497	-0.20418
Atom	C101	S102	C103	S104	C105
Charge	0.05097	-0.09030	-0.14896	-0.00045	-0.02435
Atom	S106	C107	C108	S109	H110
Charge	0.01685	-0.29732	-0.00732	0.03368	0.27859
Atom	H111	H112	H113	C114	C115
Charge	0.10387	0.28584	-0.07577	-0.03124	-0.15853
Atom	C116	C117	H118	N119	C120
Charge	0.15327	-0.50907	0.15320	0.13751	-0.11852
Atom	C121	C122	C123	C124	C125
Charge	-0.26989	0.61185	-0.54293	0.07128	0.20763
Atom	C126	C127	N128	C129	C130
Charge	-0.08830	-0.19813	0.22034	-0.06663	-0.15291
Atom	C131	C132	C133	C134	C135
Charge	-0.39216	0.22627	-0.29851	-0.07110	-0.03320
Atom	C136	C137	C138	C139	C140

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Charge	-0.05581	-0.29212	0.02685	-0.15564	-0.20799

Atom	C141	C142	C143	C144	H145
Charge	0.18919	-0.26424	-0.17023	-0.33504	0.28416
Atom	H146	H147	H148	H149	H150
Charge	0.15593	0.30503	0.20875	0.12800	0.25692
Atom	H151	H152	H153	H154	H155
Charge	0.18156	0.01272	0.22314	0.22423	0.20394
Atom	H156	H157	H158	H159	H160
Charge	0.14621	0.19120	0.17237	0.15219	0.20333
Atom	H161	H162	H163	C164	O165
Charge	0.17517	0.17608	0.20983	0.05562	-0.30327
Atom	C166	C167	O168	C169	C170
Charge	-0.06486	-0.01551	-0.31621	-0.21609	0.22335
Atom	O171	C172	C173	O174	O175
Charge	-0.46976	-0.01030	-0.09418	-0.33259	-0.06977
Atom	C176	C177	O178	C179	C180
Charge	-0.06493	-0.14787	-0.35116	-0.05135	0.08026
Atom	O181	C182	C183	O184	C185
Charge	-0.50712	0.23100	0.03900	-0.58482	0.74390
Atom	H186	H187	H188	H189	H190
Charge	0.12241	0.14776	0.13974	0.05319	0.13123
Atom	H191	H192	H193	H194	H195
Charge	0.09828	0.13927	0.15501	0.02864	0.11101
Atom	H196	H197	H198	H199	H200
Charge	0.14312	0.09784	0.14764	0.10982	0.10118
Atom	H201	H202	H203	H204	H205
Charge	0.11741	0.13270	0.15460	0.12172	0.11672
Atom	H206	H207	H208	H209	H210
Charge	0.06481	0.11334	0.11267	0.06102	0.05073
Atom	H211	H212	C213	H214	H215
Charge	0.05789	-0.02578	-0.17447	0.13051	0.16346
Atom	C216	H217	C218	C219	S220
Charge	0.04957	0.11580	-0.18729	0.01665	-0.07444
Atom	C221	S222	C223	S224	C225
Charge	-0.12622	-0.00970	-0.04632	0.01247	-0.26680
Atom	C226	S227	H228	H229	H230
Charge	-0.04640	0.05645	0.27125	0.11308	0.28012
Atom	H231	C232	C233	C234	C235
Charge	-0.04231	-0.04361	-0.15979	0.13426	-0.46061

Atom	H236
Charge	0.13678

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	0.07667	0.04287	-0.46947	0.52466	-0.54005

Atom	C6	C7	C8	C9	N10
Charge	0.12338	0.36099	-0.12112	-0.16034	0.14859
Atom	C11	C12	C13	C14	C15
Charge	0.17868	-0.48531	-0.42083	0.24361	-0.32794
Atom	C16	C17	C18	C19	C20
Charge	-0.03790	-0.04438	-0.07691	-0.27018	0.04200
Atom	C21	C22	C23	C24	C25
Charge	-0.19535	-0.14811	0.15884	-0.26555	-0.17079
Atom	C26	H27	H28	H29	H30
Charge	-0.29566	0.25049	0.17798	0.30984	0.21123
Atom	H31	H32	H33	H34	H35
Charge	0.12259	0.26530	0.02108	0.12847	0.23945
Atom	H36	H37	H38	H39	H40
Charge	0.24274	0.21296	0.13104	0.18556	0.17757
Atom	H41	H42	H43	H44	H45
Charge	0.12733	0.20713	0.17590	0.16866	0.20760
Atom	C46	O47	C48	C49	O50
Charge	0.03741	-0.27817	-0.06374	-0.01895	-0.32248
Atom	C51	C52	O53	C54	C55
Charge	-0.16357	0.14009	-0.44646	0.01039	-0.08379
Atom	O56	O57	C58	C59	O60
Charge	-0.34615	-0.10656	-0.04384	-0.18933	-0.27329
Atom	C61	C62	O63	C64	C65
Charge	-0.09093	0.07342	-0.50164	0.21683	-0.06933
Atom	O66	C67	H68	H69	H70
Charge	-0.48850	0.64756	0.12943	0.15254	0.14286
Atom	H71	H72	H73	H74	H75
Charge	0.04691	0.13567	0.09850	0.12000	0.15513
Atom	H76	H77	H78	H79	H80
Charge	0.04290	0.12777	0.13597	0.10208	0.14539
Atom	H81	H82	H83	H84	H85
Charge	0.11394	0.10622	0.12374	0.14408	0.16515
Atom	H86	H87	H88	H89	H90
Charge	0.12500	0.12973	0.05576	0.12128	0.15547
Atom	H91	H92	H93	H94	C95
Charge	0.08073	0.05008	0.08943	-0.01409	-0.20314
Atom	H96	H97	C98	H99	C100
Charge	0.15056	0.18640	0.09799	0.12643	-0.20852
Atom	C101	S102	C103	S104	C105
Charge	0.07056	0.13624	-0.12947	0.21880	-0.00583
Atom	S106	C107	C108	S109	H110
Charge	0.22298	-0.25869	-0.03751	0.17339	0.29999
Atom	H111	H112	H113	C114	C115
Charge	0.11185	0.30679	-0.04248	-0.05331	-0.11986
Atom	C116	C117	H118	N119	C120
Charge	0.09174	-0.37232	0.15299	0.13512	-0.11463
Atom	C121	C122	C123	C124	C125
Charge	-0.27573	0.61391	-0.54132	0.06869	0.21372

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Atom	C126	C127	N128	C129	C130
Charge	-0.08736	-0.19948	0.21978	-0.06345	-0.16133
Atom	C131	C132	C133	C134	C135
Charge	-0.39448	0.22703	-0.28869	-0.08998	-0.02353
Atom	C136	C137	C138	C139	C140
Charge	-0.05553	-0.29133	0.02757	-0.16205	-0.20269
Atom	C141	C142	C143	C144	H145
Charge	0.19137	-0.26736	-0.17036	-0.33208	0.28406
Atom	H146	H147	H148	H149	H150
Charge	0.15653	0.30417	0.20965	0.12776	0.25729
Atom	H151	H152	H153	H154	H155
Charge	0.18087	0.01449	0.22422	0.22541	0.20223
Atom	H156	H157	H158	H159	H160
Charge	0.15449	0.19164	0.17250	0.15230	0.20394
Atom	H161	H162	H163	C164	O165
Charge	0.17928	0.17443	0.21096	0.05672	-0.30428
Atom	C166	C167	O168	C169	C170
Charge	-0.06559	-0.01733	-0.31531	-0.21658	0.22238
Atom	O171	C172	C173	O174	O175
Charge	-0.46901	-0.01192	-0.09615	-0.33147	-0.06914
Atom	C176	C177	O178	C179	C180
Charge	-0.06513	-0.14941	-0.35091	-0.05042	0.08071
Atom	O181	C182	C183	O184	C185
Charge	-0.50699	0.22151	0.05098	-0.58447	0.72931
Atom	H186	H187	H188	H189	H190
Charge	0.12288	0.14754	0.14033	0.05393	0.13218
Atom	H191	H192	H193	H194	H195
Charge	0.09858	0.13942	0.15546	0.02876	0.11134
Atom	H196	H197	H198	H199	H200
Charge	0.14376	0.09863	0.14826	0.11093	0.10114
Atom	H201	H202	H203	H204	H205
Charge	0.11795	0.13326	0.15521	0.12199	0.11688
Atom	H206	H207	H208	H209	H210
Charge	0.06459	0.11279	0.11591	0.06357	0.04113
Atom	H211	H212	C213	H214	H215
Charge	0.05702	-0.01618	-0.17656	0.13104	0.16429
Atom	C216	H217	C218	C219	S220
Charge	0.04838	0.11645	-0.18699	0.01690	-0.07407
Atom	C221	S222	C223	S224	C225
Charge	-0.12681	-0.00879	-0.04498	0.01211	-0.26693
Atom	C226	S227	H228	H229	H230
Charge	-0.04671	0.05703	0.27141	0.11324	0.28034
Atom	H231	C232	C233	C234	C235
Charge	-0.03288	-0.04277	-0.16002	0.13537	-0.46251
Atom	H236				
Charge	0.13725				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	0.07499	0.04088	-0.47134	0.52644	-0.54340
Atom	C6	C7	C8	C9	N10
Charge	0.12059	0.37784	-0.13206	-0.16143	0.14893
Atom	C11	C12	C13	C14	C15
Charge	0.18052	-0.50821	-0.42432	0.24805	-0.32111
Atom	C16	C17	C18	C19	C20
Charge	-0.05897	-0.03424	-0.07720	-0.27035	0.04321
Atom	C21	C22	C23	C24	C25
Charge	-0.20184	-0.14267	0.16190	-0.26795	-0.17259
Atom	C26	H27	H28	H29	H30
Charge	-0.29175	0.25280	0.17347	0.30938	0.21145
Atom	H31	H32	H33	H34	H35
Charge	0.12422	0.26427	0.02209	0.13284	0.23986
Atom	H36	H37	H38	H39	H40
Charge	0.24333	0.21214	0.14133	0.18606	0.17790
Atom	H41	H42	H43	H44	H45
Charge	0.12664	0.20748	0.18041	0.16571	0.20775
Atom	C46	O47	C48	C49	O50
Charge	0.03926	-0.27816	-0.06574	-0.02080	-0.32053
Atom	C51	C52	O53	C54	C55
Charge	-0.16548	0.14237	-0.44576	0.00737	-0.08193
Atom	O56	O57	C58	C59	O60
Charge	-0.34466	-0.10796	-0.04195	-0.19183	-0.27123
Atom	C61	C62	O63	C64	C65
Charge	-0.09145	0.07566	-0.50132	0.20740	-0.06852
Atom	O66	C67	H68	H69	H70
Charge	-0.47871	0.62205	0.12967	0.15158	0.14367
Atom	H71	H72	H73	H74	H75
Charge	0.04791	0.13657	0.09878	0.12078	0.15551
Atom	H76	H77	H78	H79	H80
Charge	0.04000	0.12756	0.13712	0.10302	0.14549
Atom	H81	H82	H83	H84	H85
Charge	0.11342	0.10598	0.12401	0.14470	0.16578
Atom	H86	H87	H88	H89	H90
Charge	0.12555	0.12985	0.05497	0.12050	0.15558
Atom	H91	H92	H93	H94	C95
Charge	0.08469	0.04982	0.09042	-0.00431	-0.20234
Atom	H96	H97	C98	H99	C100
Charge	0.15121	0.18712	0.09345	0.12959	-0.20292
Atom	C101	S102	C103	S104	C105
Charge	0.07531	0.14337	-0.13364	0.22374	-0.00738
Atom	S106	C107	C108	S109	H110
Charge	0.23112	-0.25339	-0.02966	0.18032	0.30167

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Atom	H111	H112	H113	C114	C115
Charge	0.11396	0.30891	-0.02994	-0.05229	-0.12081
Atom	C116	C117	H118	N119	C120
Charge	0.09183	-0.36993	0.15391	0.17295	-0.18783
Atom	C121	C122	C123	C124	C125
Charge	-0.24390	0.55170	-0.51367	0.04880	0.16709
Atom	C126	C127	N128	C129	C130
Charge	-0.18967	-0.10000	0.17281	0.00933	-0.29677
Atom	C131	C132	C133	C134	C135
Charge	-0.40676	0.24558	-0.30623	-0.07686	-0.03515
Atom	C136	C137	C138	C139	C140
Charge	-0.04478	-0.29699	0.04005	-0.18190	-0.19945
Atom	C141	C142	C143	C144	H145
Charge	0.21050	-0.27575	-0.17170	-0.34376	0.31981
Atom	H146	H147	H148	H149	H150
Charge	0.14084	0.31122	0.22119	0.15971	0.24683
Atom	H151	H152	H153	H154	H155
Charge	0.17600	0.03389	0.22904	0.23419	0.20853
Atom	H156	H157	H158	H159	H160
Charge	0.15341	0.18886	0.17486	0.15605	0.20762
Atom	H161	H162	H163	C164	O165
Charge	0.18267	0.18180	0.21219	0.08661	-0.30806
Atom	C166	C167	O168	C169	C170
Charge	-0.08558	-0.00451	-0.34947	-0.12312	0.08251
Atom	O171	C172	C173	O174	O175
Charge	-0.44675	0.03522	-0.15232	-0.30931	-0.09370
Atom	C176	C177	O178	C179	C180
Charge	-0.07316	-0.14355	-0.34181	-0.03608	0.03461
Atom	O181	C182	C183	O184	C185
Charge	-0.48639	0.25269	-0.17489	-0.39628	0.50844
Atom	H186	H187	H188	H189	H190
Charge	0.11611	0.14424	0.14966	0.05846	0.13340
Atom	H191	H192	H193	H194	H195
Charge	0.09946	0.11192	0.15225	0.04034	0.14982
Atom	H196	H197	H198	H199	H200
Charge	0.13483	0.09916	0.16187	0.13926	0.11129
Atom	H201	H202	H203	H204	H205
Charge	0.12653	0.12747	0.15952	0.11782	0.11778
Atom	H206	H207	H208	H209	H210
Charge	0.07461	0.12604	0.11393	0.07688	0.09848
Atom	H211	H212	C213	H214	H215
Charge	0.10861	0.01764	-0.19640	0.15572	0.18524
Atom	C216	H217	C218	C219	S220
Charge	0.04776	0.14239	-0.20307	0.06315	0.14165
Atom	C221	S222	C223	S224	C225
Charge	-0.12875	0.21504	-0.01643	0.21684	-0.23258
Atom	C226	S227	H228	H229	H230
Charge	-0.06250	0.19638	0.29623	0.12733	0.30324

Atom	H231	C232	C233	C234	C235
Charge	-0.00185	-0.06186	-0.12782	0.07622	-0.32591

Atom	H236
Charge	0.13816

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	0.07376	0.05033	-0.47974	0.52486	-0.53134

Atom	C6	C7	C8	C9	N10
Charge	0.11598	0.38615	-0.12687	-0.15752	0.14755

Atom	C11	C12	C13	C14	C15
Charge	0.18505	-0.51241	-0.42580	0.25009	-0.31293

Atom	C16	C17	C18	C19	C20
Charge	-0.07852	-0.02398	-0.07644	-0.26976	0.04364

Atom	C21	C22	C23	C24	C25
Charge	-0.20540	-0.13968	0.16422	-0.27032	-0.17311

Atom	C26	H27	H28	H29	H30
Charge	-0.29091	0.25013	0.17798	0.30647	0.21291

Atom	H31	H32	H33	H34	H35
Charge	0.12306	0.26492	0.02313	0.13369	0.24130

Atom	H36	H37	H38	H39	H40
Charge	0.24507	0.20974	0.15169	0.18735	0.17793

Atom	H41	H42	H43	H44	H45
Charge	0.12686	0.20810	0.18502	0.16611	0.21008

Atom	C46	O47	C48	C49	O50
Charge	0.03893	-0.27925	-0.06442	-0.02269	-0.32199

Atom	C51	C52	O53	C54	C55
Charge	-0.16218	0.13733	-0.44519	0.00845	-0.08568

Atom	O56	O57	C58	C59	O60
Charge	-0.34470	-0.10567	-0.04328	-0.19080	-0.27205

Atom	C61	C62	O63	C64	C65
Charge	-0.09237	0.08143	-0.50078	0.19049	-0.05021

Atom	O66	C67	H68	H69	H70
Charge	-0.48320	0.60934	0.13036	0.15206	0.14364

Atom	H71	H72	H73	H74	H75
Charge	0.04816	0.13732	0.09944	0.11996	0.15541

Atom	H76	H77	H78	H79	H80
Charge	0.04315	0.12862	0.13675	0.10294	0.14594

Atom	H81	H82	H83	H84	H85
Charge	0.11533	0.10615	0.12424	0.14444	0.16581

Atom	H86	H87	H88	H89	H90
Charge	0.12628	0.13020	0.05395	0.11885	0.15367

Atom	H91	H92	H93	H94	C95
Charge	0.09090	0.04476	0.08877	0.00389	-0.20620

DOI: 10.1038/NCHEM.749

Atom	H96	H97	C98	H99	C100
Charge	0.15133	0.18751	0.09604	0.12768	-0.20916
Atom	C101	S102	C103	S104	C105
Charge	0.07181	0.13647	-0.12982	0.21957	-0.00394
Atom	S106	C107	C108	S109	H110
Charge	0.22169	-0.25918	-0.03685	0.17447	0.30031
Atom	H111	H112	H113	C114	C115
Charge	0.11184	0.30710	-0.01857	-0.04976	-0.12265
Atom	C116	C117	H118	N119	C120
Charge	0.09516	-0.37699	0.15466	0.20781	-0.25077
Atom	C121	C122	C123	C124	C125
Charge	-0.21055	0.48177	-0.47832	0.03026	0.11987
Atom	C126	C127	N128	C129	C130
Charge	-0.28808	0.00513	0.12265	0.08647	-0.42537
Atom	C131	C132	C133	C134	C135
Charge	-0.41845	0.26430	-0.32534	-0.06109	-0.04683
Atom	C136	C137	C138	C139	C140
Charge	-0.03336	-0.30251	0.05167	-0.20006	-0.19687
Atom	C141	C142	C143	C144	H145
Charge	0.22871	-0.28452	-0.17153	-0.35406	0.35091
Atom	H146	H147	H148	H149	H150
Charge	0.12599	0.31706	0.23342	0.19123	0.23635
Atom	H151	H152	H153	H154	H155
Charge	0.17099	0.05289	0.23448	0.24349	0.21501
Atom	H156	H157	H158	H159	H160
Charge	0.15182	0.18626	0.17689	0.15976	0.21157
Atom	H161	H162	H163	C164	O165
Charge	0.18584	0.18960	0.21423	0.11477	-0.31142
Atom	C166	C167	O168	C169	C170
Charge	-0.10432	0.00746	-0.38269	-0.03155	-0.05128
Atom	O171	C172	C173	O174	O175
Charge	-0.42490	0.08019	-0.20142	-0.28925	-0.12169
Atom	C176	C177	O178	C179	C180
Charge	-0.08088	-0.13541	-0.33341	-0.02155	-0.01108
Atom	O181	C182	C183	O184	C185
Charge	-0.46501	0.28063	-0.39673	-0.21327	0.29270
Atom	H186	H187	H188	H189	H190
Charge	0.10965	0.14171	0.15874	0.06285	0.13473
Atom	H191	H192	H193	H194	H195
Charge	0.10069	0.08442	0.14905	0.05059	0.18709
Atom	H196	H197	H198	H199	H200
Charge	0.12608	0.09969	0.17392	0.16499	0.12151
Atom	H201	H202	H203	H204	H205
Charge	0.13517	0.12108	0.16351	0.11383	0.11875
Atom	H206	H207	H208	H209	H210
Charge	0.08489	0.13934	0.11055	0.09100	0.15458
Atom	H211	H212	C213	H214	H215
Charge	0.16055	0.05059	-0.20860	0.17944	0.20508

Atom	C216	H217	C218	C219	S220
Charge	0.05046	0.16774	-0.21371	0.10853	0.36014
Atom	C221	S222	C223	S224	C225
Charge	-0.12880	0.44068	0.01611	0.42294	-0.19270
Atom	C226	S227	H228	H229	H230
Charge	-0.07597	0.33584	0.31966	0.14109	0.32299
Atom	H231	C232	C233	C234	C235
Charge	0.02855	-0.07905	-0.09646	0.01901	-0.19349
Atom	H236				
Charge	0.13894				

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Atomic charges from electrostatic potential:

Atom	N1	C2	C3	C4	C5
Charge	0.03960	0.09049	-0.58605	0.58131	-0.59850
Atom	C6	C7	C8	C9	N10
Charge	0.17578	0.33188	-0.18173	-0.09102	0.10645
Atom	C11	C12	C13	C14	C15
Charge	0.22242	-0.65358	-0.43042	0.27008	-0.33244
Atom	C16	C17	C18	C19	C20
Charge	-0.06691	-0.03500	-0.06344	-0.27740	0.05421
Atom	C21	C22	C23	C24	C25
Charge	-0.22249	-0.13185	0.17148	-0.27799	-0.17227
Atom	C26	H27	H28	H29	H30
Charge	-0.28742	0.27328	0.17868	0.32888	0.21186
Atom	H31	H32	H33	H34	H35
Charge	0.13979	0.26169	0.03164	0.16997	0.24588
Atom	H36	H37	H38	H39	H40
Charge	0.25206	0.21688	0.15171	0.18443	0.17849
Atom	H41	H42	H43	H44	H45
Charge	0.12696	0.21178	0.18779	0.16976	0.21137
Atom	C46	O47	C48	C49	O50
Charge	0.07320	-0.28472	-0.07916	-0.01436	-0.35313
Atom	C51	C52	O53	C54	C55
Charge	-0.09000	0.02782	-0.43299	0.04925	-0.14793
Atom	O56	O57	C58	C59	O60
Charge	-0.32634	-0.14306	-0.03701	-0.19511	-0.26048
Atom	C61	C62	O63	C64	C65
Charge	-0.07902	0.03236	-0.47958	0.22155	-0.25913
Atom	O66	C67	H68	H69	H70
Charge	-0.30108	0.38590	0.12289	0.14650	0.15195
Atom	H71	H72	H73	H74	H75
Charge	0.04842	0.13936	0.10217	0.10353	0.15352
Atom	H76	H77	H78	H79	H80
Charge	0.04916	0.16120	0.13138	0.10575	0.16178

DOI: 10.1038/NCHEM.749

Atom	H81	H82	H83	H84	H85
Charge	0.14531	0.11126	0.13100	0.14368	0.17086
Atom	H86	H87	H88	H89	H90
Charge	0.12437	0.13113	0.06601	0.13211	0.15137
Atom	H91	H92	H93	H94	C95
Charge	0.09652	0.10334	0.13650	0.03949	-0.20143
Atom	H96	H97	C98	H99	C100
Charge	0.17264	0.20431	0.10954	0.15236	-0.19923
Atom	C101	S102	C103	S104	C105
Charge	0.09782	0.35832	-0.12004	0.42947	0.01088
Atom	S106	C107	C108	S109	H110
Charge	0.42752	-0.21100	-0.05062	0.31164	0.32260
Atom	H111	H112	H113	C114	C115
Charge	0.12345	0.32799	0.01278	-0.07022	-0.08680
Atom	C116	C117	H118	N119	C120
Charge	0.03686	-0.24613	0.15438	0.20563	-0.24726
Atom	C121	C122	C123	C124	C125
Charge	-0.21572	0.48354	-0.47647	0.02760	0.12597
Atom	C126	C127	N128	C129	C130
Charge	-0.28732	0.00409	0.12232	0.08977	-0.43350
Atom	C131	C132	C133	C134	C135
Charge	-0.42064	0.26500	-0.31598	-0.07904	-0.03791
Atom	C136	C137	C138	C139	C140
Charge	-0.03325	-0.30150	0.05280	-0.20638	-0.19179
Atom	C141	C142	C143	C144	H145
Charge	0.23070	-0.28724	-0.17197	-0.35104	0.35062
Atom	H146	H147	H148	H149	H150
Charge	0.12655	0.31629	0.23444	0.19105	0.23688
Atom	H151	H152	H153	H154	H155
Charge	0.17044	0.05438	0.23557	0.24465	0.21332
Atom	H156	H157	H158	H159	H160
Charge	0.15961	0.18645	0.17709	0.15967	0.21207
Atom	H161	H162	H163	C164	O165
Charge	0.18980	0.18791	0.21518	0.11591	-0.31239
Atom	C166	C167	O168	C169	C170
Charge	-0.10446	0.00605	-0.38194	-0.03162	-0.05177
Atom	O171	C172	C173	O174	O175
Charge	-0.42447	0.07944	-0.20252	-0.28877	-0.12147
Atom	C176	C177	O178	C179	C180
Charge	-0.08047	-0.13637	-0.33312	-0.02104	-0.00989
Atom	O181	C182	C183	O184	C185
Charge	-0.46492	0.27113	-0.38280	-0.21396	0.27974
Atom	H186	H187	H188	H189	H190
Charge	0.11008	0.14140	0.15905	0.06328	0.13540
Atom	H191	H192	H193	H194	H195
Charge	0.10082	0.08455	0.14919	0.05067	0.18724
Atom	H196	H197	H198	H199	H200
Charge	0.12629	0.10002	0.17410	0.16586	0.12124

Atom	H201	H202	H203	H204	H205
Charge	0.13549	0.12154	0.16377	0.11411	0.11887
Atom	H206	H207	H208	H209	H210
Charge	0.08458	0.13850	0.11313	0.09347	0.14499
Atom	H211	H212	C213	H214	H215
Charge	0.15890	0.05951	-0.21011	0.17982	0.20577
Atom	C216	H217	C218	C219	S220
Charge	0.05008	0.16808	-0.21341	0.10887	0.36061
Atom	C221	S222	C223	S224	C225
Charge	-0.12910	0.44162	0.01712	0.42282	-0.19296
Atom	C226	S227	H228	H229	H230
Charge	-0.07627	0.33558	0.31972	0.14093	0.32314
Atom	H231	C232	C233	C234	C235
Charge	0.03719	-0.07835	-0.09657	0.01955	-0.19487
Atom	H236				
Charge	0.13936				